PB85-160356

Testing and Evaluation of TOX-SCREEN Model

Anderson-Nichols and Co., Inc., Palo Alto, CA

Prepared for

Environmental Research Lab., Athens, GA

Jan 85

U.S. Department of Commerce
National Technical Information Service
NTIS

PB85-160356

EPA/600/3-85/001
January 1985

TESTING AND EVALUATION OF TOX-SCREEN MODEL

by

Brian R. Bicknell
Scott H. Boutwell
David B. Watson

Anderson-Nichols & Co., Inc.
Palo Alto, CA 94303

Contract No. 68-03-3116

Project Officer
Lee A. Mulkey
Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30613

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GA 30613

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/3-85/001	2.	3. RECIPIENT'S ACCESSION NO. PB85 160356/AS
4. TITLE AND SUBTITLE Testing and Evaluation of TOX-SCREEN model		5. REPORT DATE January 1985
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Brian R. Bicknell, Scott H. Boutwell and David B. Watson		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Anderson-Nichols & Co., Inc. Palo Alto CA 94303		10. PROGRAM ELEMENT NO.
		11. CONTRACT/GRANT NO. 68-03-3116
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency--Athens GA Office of Research and Development Environmental Research Laboratory Athens GA 30613		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE EPA/600/01

15. SUPPLEMENTARY NOTES

16. ABSTRACT

The TOX-SCREEN model, which was developed recently by the U.S. EPA Office for Toxic Substances, is a screening level, multimedia model designed to provide rapid assessment of the long-term tendency of toxic chemicals to accumulate in air, surface water, and soil. TOX-SCREEN simulates pollutant fate and transport by considering the release and dispersion of chemicals into the air, water, and soil; atmospheric deposition; volatilization; adsorption; leaching; and chemical-biological degradation. Transport of pollutants across media interfaces is specified by atmospheric deposition velocities, mass transfer coefficients, and mass loading parameters. The model assumes a generic positioning of surface water bodies and contaminated land areas with respect to atmospheric pollutant sources.

In this study, an evaluation of TOX-SCREEN to determine its ability to perform reliable screening of chemicals was conducted. Evaluation included a review of the TOX-SCREEN processes and models relative to the current state-of-the-art methods, a comparison of TOX-SCREEN results with observed data and with predictions of other models, and a sensitivity analysis of selected input parameters.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 137
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (9-73)

DISCLAIMER

The information in this document has been funded by the United States Environmental Protection Agency. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use by the U.S. Environmental Protection Agency.

FOREWORD

As environmental controls become more costly to implement and the penalties of judgement errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops management and engineering tools to help pollution control officials achieve water quality goals through watershed management.

The TOX-SCREEN model simulates pollutant fate and transport in and between air, soil, and surface water. Since its completion, the model has undergone only limited testing. This report describes a more thorough evaluation of the ability of TOX-SCREEN to screen chemicals and identify those that are unlikely to pose significant risk. The evaluation includes the identification of a number of improvements that would allow the model to be applied to a wider spectrum of chemicals.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

The TOX-SCREEN model, which was recently developed for the U.S. Environmental Protection Agency's Office of Toxic Substances by Oak Ridge National Laboratory, is a screening level, multimedia model designed to provide rapid assessment of the long-term tendency of toxic chemicals to accumulate in air, surface water, and soil. TOX-SCREEN simulates pollutant fate and transport by considering release and dispersion of chemical into the air, water, and soil; atmospheric deposition; volatilization; adsorption; leaching; and chemical-biological degradation. Transport of pollutants across media interfaces is specified by atmospheric deposition velocities, mass transfer coefficients, and mass loading parameters. The model assumes a generic positioning of surface water bodies and contaminated land areas with respect to atmospheric pollutant sources.

In this study, an evaluation of TOX-SCREEN to determine its ability to perform reliable screening of chemicals was conducted. Evaluation included a review of the TOX-SCREEN models and processes relative to the current state-of-the-art methods, comparison of TOX-SCREEN relsults with observed data and with predictions of other models, and a sensitivity analysis of selected input parameters.

This work was submitted in partial fulfillment of Contract No. 68-03-3116 by Anderson-Nichols and Co., Inc., under the sponsorship of the U.S. Environmental Protection Agency. This report covers a period from May 7, 1982, to September 30, 1984, and work was completed as of September 30, 1984.

CONTENTS

Page

Abstract.. iii
Figures... vii
Tables.. ix
Acknowledgments................................. xi
1.0 Introduction................................ 1
    1.1 Project Background and Objective........ 1
    1.2 Overview of TOX-SCREEN.................. 3
    1.3 Overview of Testing Procedures.......... 5
    1.4 Report Organization..................... 6
2.0 Atmospheric Model........................... 7
    2.1 Review and Evaluation by H.E. Cramer Co... 7
    2.2 Response to Air Model Evaluation by Oak Ridge Laboratory.................... 13
    2.3 Previous Testing Results................ 15
    2.4 Sensitivity Testing..................... 19
    2.5 Conclusions............................. 29
3.0 Soil Model.................................. 32
    3.1 Review and Evaluation................... 32
    3.2 Previous Testing Results................ 39
    3.3 Current Testing Results................. 43
4.0 Aquatic Models.............................. 45
    4.1 Review and Evaluation................... 45
    4.2 Previous Testing Results................ 53
    4.3 Current Testing Results................. 57
    4.4 Conclusions............................. 75
5.0 Intermedia Transfer......................... 77
    5.1 Review and Evaluation................... 77
    5.2 Sensitivity Testing..................... 86
    5.3 Conclusions............................. 87
6.0 Application of TOX-SCREEN to Southeast Ohio Study Area............................. 94
    6.1 Description of SEOSA and Data Base...... 94
    6.2 Model Application....................... 97
7.0 TOX-SCREEN Code and Documentation........... 109
    7.1 Code.................................... 109
    7.2 Documentation........................... 110
    7.3 Input................................... 111
    7.4 Output.................................. 112

8.0 Conclusions and Recommendations................ 113
    8.1 Suitability of TOX-SCREEN for Screening... 113
    8.2 Recommended Changes....................... 114
References.. 117

FIGURES

Page

1.1 Pollutant pathways simulated in TOX-SCREEN....... 4

2.1 Sensitivity of air pollutant concentrations to stack height.................................... 22

2.2 Sensitivity of air pollutant concentrations to stack radius.................................... 23

2.3 Sensitivity of air pollutant concentrations to mixing height.................................... 24

2.4 Sensitivity of air pollutant concentrations to gravitational settling velocity................. 25

2.5 Sensitivity of air pollutant concentrations to stack gas exit velocity......................... 26

2.6 Sensitivity of air pollutant concentrations to stack gas enthalpy.............................. 27

2.7 Sensitivity of air pollutant concentrations to stack gas density............................... 28

4.1 Comparison of TOX-SCREEN with EXAMS, HSPF, and WASP - Chemical 1................................ 62

4.2 Comparison of TOX-SCREEN with EXAMS, HSPF, and WASP - Chemical 2................................ 63

4.3 Ammonia-N concentrations in the Mississippi River - comparison of model results and observed data.................................. 66

4.4 Dissolved Dieldrin in Saylorville Reservoir - comparison of TOX-SCREEN to observed data........ 70

4.5 Total Dieldrin in Saylorville Reservoir - comparison of TOX-SCREEN to observed data........ 71

4.6 Non-conservative pollutant in Newport Bay Estuary - comparison of TOX-SCREEN to link-node model.... 74

5.1 Generic environment for atmospheric point source, river, and soil........................ 83

5.2 Generic environment for atmospheric point source, lake, and soil......................... 84

5.3 Atmospheric area source generic environment in TOX-SCREEN showing pollutant movement............ 85

5.4 Sensitivity of atmospheric deposition to dry deposition velocity (washout ratio = 0).......... 89

5.5 Sensitivity of atmospheric deposition to dry deposition velocity (washout ratio = 5.E+5)...... 90

5.6 Sensitivity of atmospheric deposition to washout ratio (dry deposition velocity = 0).............. 91

5.7 Sensitivity of atmospheric deposition to washout ratio (dry deposition velocity = 1 cm/s)......... 92

6.1 Southeast Ohio study area....................... 95

6.2 Comparison of observed and simulated air concentrations of benzo(a)pyrene in the Southeast Ohio study area....................... 108

TABLES

Page

2.1 Input Parameters For Previous Air Model Tests.................................... 16

2.2 Input Parameters and Results of Previous Air Model Tests.................................... 17

2.3 Input Parameters for Air Model Sensitivity Tests.................................... 20

2.4 Values of Test Parameters for Air Model Sensitivity Analysis.......................... 21

3.1 Processes Simulated By the TOX-SCREEN Version of SESOIL.................................... 34

3.2 Comparison of SESOIL Predictions With Measured Pollutant Concentrations at Two Land Treatment Sites.............................. 41

4.1 Input Parameters for TCE Tests................. 55

4.2 Input Parameters and Results of TCE Testing..... 56

4.3 Scenarios Tested with TOX-SCREEN Aquatic Models. 58

4.4 Parameter Values for Yazoo River Tests.......... 60

4.5 River Velocities for Yazoo River Tests.......... 61

4.6 Parameter Values for the Mississippi River (RM170) Test.................................. 65

4.7 Parameter Values for the Saylorville Reservoir Test................................ 68

4.8 Monthly Loading Rates of Dieldrin into Saylorville Reservoir........................... 69

4.9 Parameter Values for Newport Bay Estuary Tests.. 73

5.1 Values of the Test Parameters for Sensitivity Tests of Atmospheric Deposition................ 88

6.1 Model Flags and Air Compartment Input for SEOSA Application.. 98

6.2 River Compartment Input for SEOSA Application... 99

6.3 Soil Compartment Input (Hydrologic Parameters) for SEOSA Application........................... 100

6.4 Soil Compartment Input (Soil and Chemical Parameters) for SEOSA Application............... 101

6.5 Benzo(a)pyrene Concentrations Predicted for Southeast Ohio Study Area....................... 104

6.6 Benzo(a)pyrene Intermedia Fluxes Predicted for Southeast Ohio Study Area....................... 105

6.7 Measured Benzo(a)pyrene Concentrations in the Southeast Ohio Study Area....................... 107

ACKNOWLEDGMENTS

Testing of the TOX-SCREEN model described in this report was performed as Work Assignment No. 8 of Contract No. 68-03-3116 for the U.S. Environmental Protection Agency Office of Research and Development. Mr. Lee A. Mulkey of the Environmental Research Laboratory in Athens, Georgia was the Project Officer.

Among the authors, Mr. Brian R. Bicknell was responsible for the overall project management and the sections on intermedia transfer and the model application to the Southeastern Ohio data set. Mr. Scott H. Boutwell was primarily responsible for the aquatic model evaluations. Mr. Dave B. Watson wrote the soil model section, and assisted in data collection and analysis for the model application.

Mr. James Bowers of H.E Cramer Co. Inc, Salt Lake City, Utah prepared the initial review of the air dispersion model. Mr. Dave Hetrick of Oak Ridge National Laboratories provided TOX-SCREEN documentation and testing results. Mr. John L. Kittle assisted in the TOX-SCREEN code review. Technical guidance and review were provided by Mr. Anthony S. Donigian, Jr. and Mr. Stuart M. Brown. Drafting and graphics were prepared by Ms. Virginia Rombach, and Ms. Carol McCullough assisted with the word processing.

SECTION 1

INTRODUCTION

1.1 PROJECT BACKGROUND AND OBJECTIVE

The Toxic Substances Control Act (TSCA) of 1976 requires that EPA evaluate the risks associated with the manufacture and use of chemicals. Additionally, implementation of a number of other environmental control statutes, such as the Clean Water Act, the Clean Air Act, the Safe Drinking Water Act, and the Federal Insecticide, Fungicide, and Rodenticide Act implicitly require an assessment of health risks posed to humans and other life by the manufacture and use of chemicals. One of the effects of these statutes has been to focus attention on multimedia (i.e., air, water, soil, and biota) considerations in chemical risk assessments.

Pollutants are often released to more than one medium or portion of the environment, and also may be transferred between media. Thus significant effects may occur in more than one medium or may be more important in a medium other than the one to which the pollutant was released. Consequently, a number of multimedia chemical fate and exposure methodologies have been developed to assist in the risk assessment activities mandated by the environmental control statutes. Generally, these methodologies have been "constructed" by linking separate chemical fate/transport models for single media and effecting intermedia transfers by deposition, volatilization, runoff, and erosion process models.

The TOX-SCREEN model was developed for EPA Office of Toxic Substances (OTS) to provide a multimedia, screening level model designed to enable rapid assessment of the long-term tendency of toxic chemicals to accumulate in air, surface water, soil, and ultimately in biota. Because TOX-SCREEN was designed to be a screening tool for evaluating chemicals, it is simplified to minimize input requirements, and it is designed to be overly predictive or conservative. TOX-SCREEN estimates pollutant concentrations in the various media based on chemical property data, climatic and soil data, simple water body descriptions, and the chemical release scenario.

1.1.1 TOX-SCREEN Usage by EPA Office of Toxic Substances

To better understand the original intended use of TOX-SCREEN and why it was developed, we contacted EPA Office of Toxic Substances. The following discussion is based on OTA (1983) and personal communication with R. Kinerson (1983).

In a premanufacture notification (PMN) evaluation of a proposed chemical, OTS first performs an overview or preliminary analysis in which a number of disciplines analyze all available data for the chemical. An interdisciplinary group of biologists, chemists, and toxicologists performs a structure-activity analysis; they evaluate all the anticipated properties and toxic effects (at various concentrations) based on analogous compounds and data submitted by the chemical company. An engineering group evaluates the manufacturing and processing activities to determine likely modes and amounts of releases to the environment. Another group evaluates potential releases caused by consumer uses of the compound.

Based on a consensus of these evaluations, the chemical is categorized as (1) likely to pose significant risk, (2) risks are possible, or (3) unlikely to pose significant risks. Chemicals in the first category may then undergo a "detailed review" in which fate/exposure modeling is utilized to determine the extent and type of risk posed. TOX-SCREEN is employed in the initial stages of modeling, primarily to identify the pathways and media most likely to be significant for the chemical of interest.

TOX-SCREEN is executed using chemical property data and release data developed in the initial evaluation efforts and provided by the manufacturer. Climatic and soil data are chosen which are representative of the areas of the country identified as the most likely to have greatest production and use of the chemical.

Model estimates of upper-bound chemical concentrations in the various media are compared with "risk" concentrations determined in initial evaluations. If the TOX-SCREEN estimates are not at least two orders of magnitude below the risk concentrations, then a more detailed analysis is indicated, using more sophisticated models for specific environmental media. These models include ATM for air

(Culkowski and Patterson, 1976); EXAMS for aquatic environments (Burns et al., 1982); SESOIL for soil (Bonazountas and Wagner, 1981), and UTM-TOX for multimedia applications (Patterson et al., undated).

TOX-SCREEN was developed by personnel at Oak Ridge National Laboratory Health and Safety Research Division. Documentation of the model algorithms (McDowell-Boyer and Hetrick, 1982), was published in June 1982 and a user's manual (Hetrick and McDowell-Boyer, 1984) was published in June 1984. Limited testing of the program has been accomplished since completion of the model.

The objective of this work is to conduct a thorough evaluation of TOX-SCREEN for its ability to "screen chemicals and identify those which are unlikely to pose significant risk". Evaluation methods include detailed review of model algorithms, comparison with actual data, and comparison with other models.

1.2 OVERVIEW OF TOX-SCREEN

TOX-SCREEN simulates pollutant transport and fate in and between air, soil and surface water. Point and area sources of pollutant are considered for atmospheric dispersion. The soil model simulates hydrology and pollutant transport/fate in a soil column between the ground surface and the upper saturated soil zone. Surface water bodies modeled are rivers, lakes, estuaries, and ocean outfall areas. The pollutant fate and transport processes simulated in TOX-SCREEN are shown schematically in Figure 1.1.

Implementation of the TOX-SCREEN program was accomplished by linking separate code sections for air, soil and aquatic processes. The air model uses a modified Gaussian plume equation for dispersion from a point source and a simple box model for an area source. Pollutant degradation is considered. The soil model uses Level 3 of the Seasonal Soil (SESOIL) model (Bonazountas and Wagner, 1981); SESOIL considers rainfall, infiltration, surface runoff, evapotranspiration, ground-water runoff, sediment erosion by wind and water, and chemical fate/transport processes. The aquatic models (river, lake, etc.) assume a completely mixed water body, advection of pollutant with water, pollutant interactions/decay, and adsorption to suspended sediments.

Physical and chemical processes drive transport of pollutants across air-soil and soil-water interfaces. These media

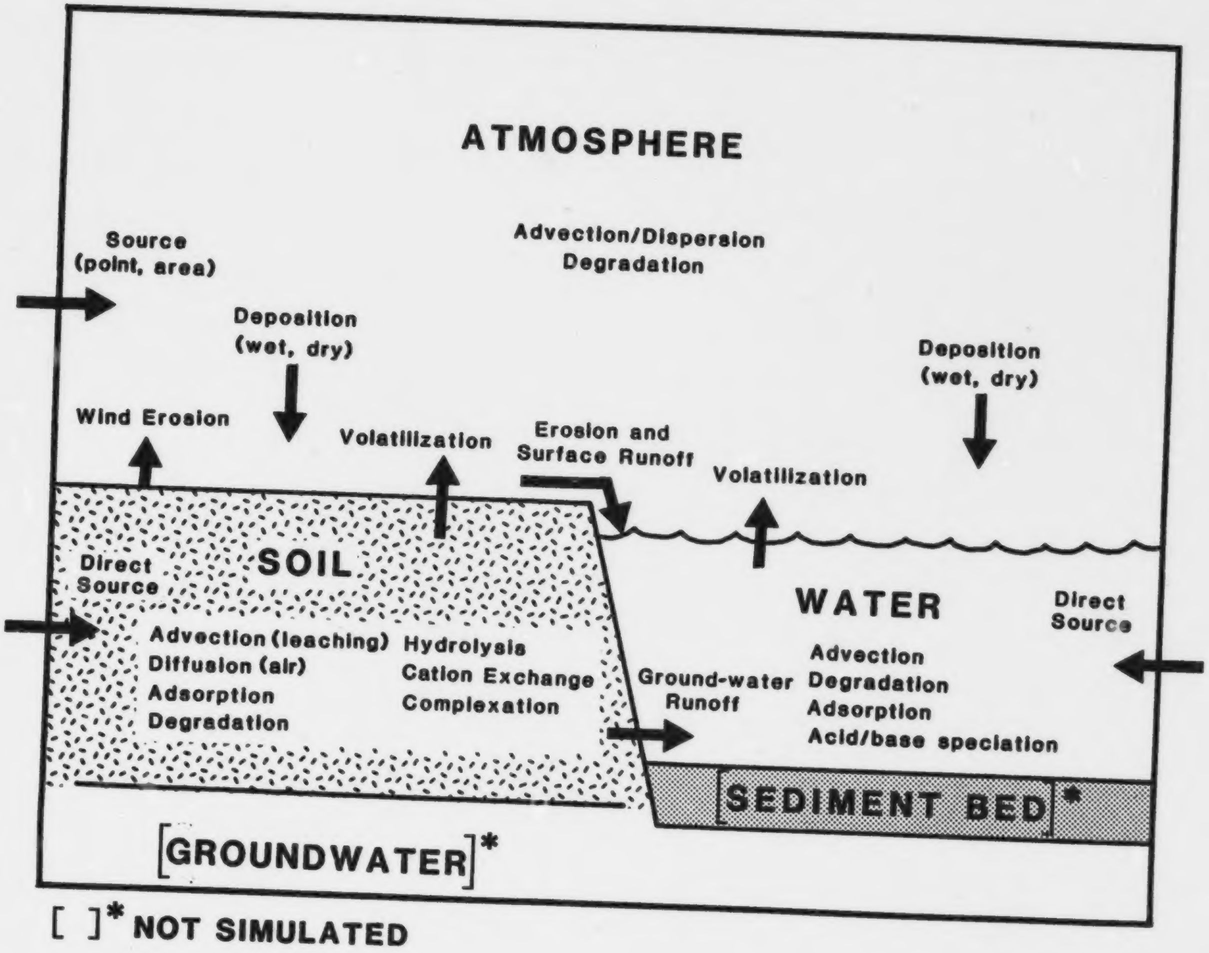

Figure 1.1 Pollutant Pathways Simulated in TOX-SCREEN

interactions (shown in Figure 1.1 as arrows) occur in TOX-SCREEN via such processes as volatilization from water and soil surfaces, wind resuspension, atmospheric deposition, surface and subsurface runoff, and soil erosion. Estimation of pollutant fluxes across media interfaces also requires the locations of water bodies relative to atmospheric pollutant sources and contaminated land areas. In TOX-SCREEN, a generic positioning of media is assumed in which the contaminated soil area is always adjacent to any water body. Water bodies are assumed to intercept the atmospheric pollutant plume almost immediately downwind of the maximum concentration point. If no water body is simulated, the land area immediately downwind of this point is assumed to be the contaminated soil area.

Pollutant concentrations in the three media reflect both direct input to any or all of the media from specified source(s), and subsequent interaction via the processes listed above. TOX-SCREEN simulates a one year period during which pollutant source terms and environmental driving forces (wind speed, velocity, rainfall, etc.) may vary monthly. During a time step (month), the source terms are assumed to be constant.

1.3 OVERVIEW OF TESTING PROCEDURES

The procedures used for evaluating TOX-SCREEN were generally motivated by two concepts. First, the multimedia nature of TOX-SCREEN raises the question of testing processes in several media concurrently or individually. Lack of comprehensive multimedia data with which to test models of this type is a problem. Separate testing of component models, including the intermedia transport models, is the alternative. Second, the screening nature of TOX-SCREEN and its "conservatism" complicate comparison testing with observed data. Generally, environmental screening level models are expected to be accurate to within approximately one order of magnitude (EPA, 1982). In addition to the simplifications incorporated into TOX-SCREEN, intentional conservatism was also incorporated which may tend to make its predictions even less accurate when compared to observed pollutant concentrations. Thus validation of the model by standard field testing methods must consider these caveats.

As a result of the above problems, TOX-SCREEN testing procedures were based primarily on 1) the individual process models (intramedia and intermedia) rather than comprehensive multimedia testing; and 2) review/evaluation of model algorithms. Comparison with observed data and other models was performed, but the overall evaluation relied more on objective evaluations of the model components, comparison with simple, idealized models, and sensitivity testing. In summary, the procedures utilized in this project to evaluate TOX-SCREEN were the following:

1) Review the transport/transformation models in detail for each environmental medium (air, soil, water) and the media interaction models (runoff, volatilization, deposition, etc.); compare with other models and state-of-the-art methods for the processes; identify major assumptions, deficiencies, etc.

2) Compare predictions of individual media models with observed data (where available) and other model predictions recognizing the temporal and spatial simplifications of TOX-SCREEN

3) Perform sensitivity testing of selected input parameters. This was performed primarily for the atmospheric model and atmospheric deposition parameters

1.4 REPORT ORGANIZATION

This report is organized by the individual media or component models which make up TOX-SCREEN. They are: the atmospheric dispersion model (Section 2), soil model (Section 3), aquatic models (Section 4), and the intermedia transfer models (Section 5). Each of these sections contains (1) a description of the model processes and algorithms, (2) evaluation of the model including comparison with state-of-the-art methods and the major limitations and assumptions, and (3) description of model testing and resulting conclusions, including earlier model testing work.

Section 6 consists of a description of TOX-SCREEN tests using a multimedia data set from the Southeast Ohio Study Area (SEOSA). Section 7 is an evaluation of the TOX-SCREEN program with regard to code structure, programming methods, documentation, input formats, output content and formats, and documentation. Section 8 presents the key overall conclusions of the TOX-SCREEN evaluation/testing and recommendations for use of the model and possible modifications.

SECTION 2

ATMOSPHERIC MODEL

2.1 REVIEW AND EVALUATION BY H.E. CRAMER CO.

Under contract to Anderson-Nichols, H.E. Cramer Co., Inc. reviewed the atmospheric dispersion/deposition model component of TOX-SCREEN because of their knowledge and expertise in this field. Their evaluation - in the form of a 'Technical Note' - is reproduced below (HEC, 1983).

The purpose of this Technical Note is to provide the H.E. Cramer Company's answers to the following specific questions from Anderson-Nichols about the atmospheric dispersion/deposition model component of the TOX-SCREEN model:

1) How does the model compare with state-of-the-art methods for simulating pollutant concentrations and deposition to water and soil?

2) What are the important deficiencies/disadvantages of the model?

3) Is the model appropriate for screening chemicals?

4) What degree of conservatism does the model afford?

Additionally, this Technical Note provides recommendations on how the dispersion/deposition component of the TOX-SCREEN model might be further evaluated by Anderson-Nichols. We caution that the description of the TOX-SCREEN model given in McDowell-Boyer and Hetrick (1982) (abbreviated as MBH) is at times ambiguous and lacking in detail. Consequently, it is possible that some of our comments may not accurately characterize the TOX-SCREEN model.

2.1.1 Model Description

The TOX-SCREEN model calculates concentration and deposition attributable to emissions from a stack using a steady-state Gaussian Plume model, which includes a tilted plume modeling approach when applied to particulate emissions with appreciable gravitational settling velocities. Plume rise is calculated using an updated version of an adiabatic plume rise equation given by Briggs (1969). The short-term ground-level concentration pattern is assumed to apply for as long as a year, (i.e., wind direction is constant in TOX-SCREEN) although wind speed may be varied from one month to the next.

The model does not consider the variation of wind speed with height. The Briggs (1973) rural dispersion coefficients (after conversion to Gaussian form) for the neutral Pasquill D stability category are used in the model calculations. Chemical transformations are accounted for by a time-dependent exponential decay term which corresponds to a pseudo-first-order reaction mechanism.

Wet deposition is parameterized by the washout ratio and monthly precipitation, and dry deposition is parameterized by the dry deposition velocity. Different deposition rates can be assigned to particulates and gases. The restriction on vertical plume growth at the top of the surface mixing layer is accounted for by specifying a maximum value for the vertical dispersion coefficient σ_z. This limit on σ_z is related to the mixing height and the plume stabilization height.

The calculated maximum short-term ground-level concentration apparently is assumed to represent the pollutant's long-term ambient air quality impact. To obtain the ground-level concentrations available for wet and dry deposition to soil and water, the crosswind-integrated concentration is divided by $4\,\sigma_y$, where σ_y is the lateral dispersion coefficient. The crosswind-integrated concentration is also averaged over the distance between the maximum ground-level concentrations x(max) and the maximum downwind distance of interest to the user x(final). Thus, the deposition calculations assume a rectangular concentration distribution within $\pm 2\sigma_y$ of the plume centerline in the interval from x(max) to x(final). The Gifford and Hanna (1973) semi-empirical ATDL area source model is used to account for emissions from: (1) directly contaminated soil, and (2) resuspension from soil and volatilization from soil and water of the deposited pollutant. The area source apparently covers the entire area of concern for the screening calculations.

2.1.2 Consistency with the State-of-the-Art Models

The atmospheric dispersion/deposition model component of the TOX-SCREEN model is a simplified version of current state-of-the-art Gaussian dispersion models such as the EPA Single Source (CRSTER) Model (EPA, 1977) and the EPA Industrial Source Complex (ISC) Dispersion Model (Bowers et al., 1979). The major technical differences between these regulatory models and the TOX-SCREEN model are: (1) the regulatory models use Pasquill-Gifford dispersion coefficients (Turner, 1970) rather than Briggs (1973) rural dispersion coefficients, (2) the regulatory models account for the variation of wind speed with height, (3) the regulatory models use the method for image sources to account for the restriction on plume growth at the top of the surface mixing layer, (4) the regulatory models do not attempt to account for wet or dry deposition except that the ISC Model can account for dry deposition of particulates but not gases, (5) the regulatory models use more advanced versions of the Briggs plume rise equations, and (6) the regulatory models either do not have area source algorithms or have area source algorithms that are more complex than the Gifford and Hanna (1973) model. The differences between the TOX-SCREEN model and the regulatory models in part tend to bias the predictions of the TOX-SCREEN model towards overestimation of long-term impacts (for example, the assumption of a constant wind direction) and in part are required to enable the TOX-SCREEN model to address intermedia transfer (for example, wet and dry deposition). The parameterizations by the TOX-SCREEN model of wet and dry deposition are of the forms used by the current research-grade long-range transport models (see Bass, 1980). Deficiencies and disadvantages of the dispersion/deposition model component of the TOX-SCREEN model are discussed below.

2.1.3 Important Deficiencies/Disadvantages

The major deficiencies of the TOX-SCREEN model are: (1) the plume rise equations are incorrectly used and can be simplified, (2) the formulation for the buoyancy flux can be made more convenient for the user, (3) the technique used to estimate the maximum value of the vertical dispersion coefficient may in some cases underestimate ground-level concentrations, (4) the guidance on the selection of the Holzworth (1972) mixing heights is inappropriate, and (5) mass continuity is not necessarily maintained.

The TOX-SCREEN model uses the adiabatic plume rise algorithms given by Equations (4.34) and (4.35) of Briggs (1969) with the coefficient 1.8 redefined as 1.6 to reflect more recent data (Briggs, 1972). Equation (2-7) in MBH apparently is used by the TOX-SCREEN model at all downwind distances beyond the distance x*. According to Briggs (1969, p. 46) this equation should not be applied beyond 5x*. Briggs (1969, p. 47) further notes that the combination of Equations (4.34) and (4.35), which correspond to Equations (2-6) and (2-7) in MBH, does not fit the available plume rise data at and beyond a downwind distance of 10Hs as well as Equation (2-6) in MBH with (x)**2/3 replaced by (10Hs)**2/3, where Hs is the physical stack height. For the vertical dispersion coefficient used by the TOX-SCREEN model, the maximum ground-level concentration is unlikely to occur at a downwind distance less than the distance to final plume rise (10Hs). Thus, there is no need for the use of a distance-dependent plume rise equation and the TOX-SCREEN model can be both simplified and made more accurate by the replacement of Equations (2-6) and (2-7) in MBH with:

$$\Delta H = 1.6\ F^{1/3} \cdot (\bar{u})^{-1} \cdot (10H_s)^{2/3} \qquad (2.1)$$

where F is the buoyancy flux and u is the mean wind speed. The current version of the TOX-SCREEN model must use an iterative approach to identify the location of the maximum ground-level concentration because of the distance dependence of the effective stack height H, which is equal to the sum of Hs and ΔH. If Equation (2.1) is implemented in the TOX-SCREEN model, the distance to the maximum ground-level concentration can readily be obtained from the expression:

$$x_{max} = \frac{H}{\sqrt{2}\sigma_e'} \qquad (2.2)$$

where σ_e is a dimensionless vertical turbulence intensity equal to .0465 for a D stability category and rural conditions.

The TOX-SCREEN model relates the buoyancy flux F to the stack radius r, stack exit velocity w, stack gas density ρg and enthalpy of the stack gas. Appendix A in MBH gives the enthalpies of various gases (CO_2, N_2, O_2, H_2O, and air) and the density of air ρ_a as a function of temperature. We believe that a more convenient expression for F is (Briggs, 1969, p. 28):

$$F = gr^2w(1-\rho_g/\rho a) \tag{2.3}$$

where g is the acceleration due to gravity. Under the assumption that the molecular weights of air and the stack gas are approximately the same (the TOX-SCREEN model's default assumption), Equation (2.3) reduces to:

$$F = gr^2w(1-T_a/T_s) \tag{2.4}$$

where T_a is the ambient air temperature and T_s is the stack gas temperature. Virtually all state-of-the-art dispersion models use Equation (2.4).

To account for the limit on vertical mixing at the top of the surface mixing layer, the TOX-SCREEN model does not allow the vertical dispersion coefficient σ_z to exceed the value given by:

$$\sigma_z(\text{limit}) = \frac{2(H_{\text{lid}}-H)}{2.15} \tag{2.5}$$

where H_{lid} is the mixing height. The vertical dispersion coefficient appears in the vertical term of the concentration equation as:

$$\exp\left[-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2\right] \tag{2.6}$$

Comparison of Equations (2.5) and (2.6) shows that, in the limit as H approaches H_{lid}, the vertical term approaches zero. In other words, the TOX-SCREEN model will not allow a plume that stabilizes near the top of the surface mixing layer to mix to the surface. There are three possible solutions to this problem. The first and most accurate solution is to incorporate a vertical term which accounts for reflection at the top of the surface mixing layer (see Section 2 of Bowers et al. (1979) for a more detailed discussion), the second solution is to set σ_z (limit) equal to $0.8 * H_{\text{lid}}$ and the third solution is to interpolate from unrestricted vertical mixing to uniform vertical mixing using the technique outlined by Turner (1970, p. 36).

According to MBH (p. 10), the current Guideline on Air Quality Models (EPA, 1978) "recommends that the mean annual afternoon mixing height from Holzworth (1972) be used for H_{lid} for a D stability category." This statement is incorrect; the Guideline does not provide any specific guidance on mixing heights. Because of the diurnal variation of mixing heights, the use in the TOX-SCREEN model of mean annual afternoon mixing heights will result in a bias toward underestimation of ground-level concentrations and deposition at the longer downwind distances. In our opinion, a more appropriate mixing height for use with the TOX-SCREEN model is the average of the mean annual early morning and afternoon mixing heights.

It is not clear from the discussion in MBH of the procedures used by the TOX-SCREEN model to account for the resuspension and volatilization of the deposited pollutant that mass continuity is preserved. For example, we have found no checks in MBH to ensure that the amount of material resuspended does not exceed the amount of material deposited. If there is a failure to preserve mass continuity, the relative apportionment of the pollutant in air, water and soil may be in error.

2.1.4 Appropriateness for Screening Chemicals

Until the effects of the above deficiencies/disadvantages are further investigated by sensitivity analyses (see Section 3), the appropriateness of the TOX-SCREEN model for screening chemicals remains open to question. Assuming the mass continuity and the deficiencies that are discussed above are addressed, we know of no reason that precludes the use of the model for screening chemicals.

2.1.5 Degree of Conservatism in the Model

One definite bias toward overestimation in the dispersion/deposition model component of the TOX-SCREEN model is the assumption that the short-term concentration pattern for a single wind direction is applicable for long-term average concentrations. The neglect of the height dependence of wind speed also results in a bias toward overestimation. The remaining dispersion/deposition model assumptions do not have any definite bias toward underestimation or overestimation of long-term impacts. Thus, the conservatism in the TOX-SCREEN model is primarily related to the "worst-case" source-receptor relationship and the constant wind-direction assumption.

2.1.6 Recommendations for Further Model Evaluation

It is not widely recognized outside of the dispersion modeling community that the data required to evaluate and verify dispersion models generally are not available. The data sets cited in the current scientific literature generally were collected for regulatory purposes and lack the necessary detail for model testing or were collected to study unique problems such as the effects of aerodynamic building wakes on the dispersion of emissions from building vents.

In the absence of data suitable for testing the atmospheric dispersion/deposition model component of the TOX-SCREEN model, we recommend that Anderson-Nichols conduct sensitivity analyses of the interactions between various parameters such as dry deposition velocities and washout ratios. (The review paper by McMahon and Denison (1979) provides a good summary of the ranges of deposition velocities and washout ratios estimated from field and laboratory measurements). The purpose of these sensitivity analyses is to determine the extent to which variations in wet and dry deposition parameters affect the relative accumulation of a pollutant in the air, soil and water and to identify any systematic biases that may be introduced by the models default parameters. We also recommend that the TOX-SCREEN model be executed under the assumption of no chemical conversions (a "chemical degradation constant" k equal to zero) to determine whether the sum of the pollutant contained in the air, water and soil equals the amount of the pollutant emitted. The TOX-SCREEN model is a unique screening model, and we are not aware of any similar model with which it can be compared. Also, even if there is a similar model, the data base needed to evaluate the accuracy of the predictions of the two models does not, to our knowledge, exist.

2.2 RESPONSE TO AIR MODEL EVALUATION BY OAK RIDGE LABORATORY

Oak Ridge National Laboratory personnel prepared a response to H.E. Cramer's evaluation of the TOX-SCREEN atmospheric model (ORNL, 1983). That response is reproduced below.

A review of the atmospheric model component of the TOX-SCREEN model has been prepared by H.E. Cramer Company Inc. (Salt Lake

City, Utah) for Anderson-Nichols and Co., Inc. (Palo Alto, California). This was done as part of the evaluation being performed by Anderson-Nichols and Co., Inc. for the EPA Environmental Research Laboratory in Athens, Georgia. Please find this Technical Note enclosed. We have read the review and have the following comments.

First, the review states....that "the difference between the TOX-SCREEN model and the regulatory models in part tend to bias the predictions of the TOX-SCREEN model toward overestimation of long-term impacts..." We agree that the TOX-SCREEN model will usually predict higher concentrations in the air compartment than the regulatory models, but this statement makes the assumption that the regulatory models are right. Of course, this is not necessarily always the case. Whether TOX-SCREEN "overestimates" in long-term impacts can be debated in certain situations, even though it should be considered a conservative model.

Second, it is stated in item (1) under Important Deficiences/Disadvantages that the plume rise equations are incorrectly used. This is not true. Briggs (1969) does state that the equation used in TOX-SCREEN "should not be applied beyond x=5x* because so few data go beyond this distance." However, the equation that H.E. Cramer Company, Inc. recommends (Equation 2.1) also has its limitations. Briggs (1969, p. 47) states "Because of the nature of the approximation used in Equation 5.1 (Eqn. 2.1 above) and the scarcity of the data beyond x=5x*, Equation 5.1 is recommended as an alternative to Equation 4.34 (the equation used in TOX-SCREEN) only for fossil-fuel plants with a heat emission of at least 20 Mw at full load". Although the method recommended by H.E. Cramer Company, Inc. is simpler to use than the one previously employed by TOX-SCREEN, we note that the iterative approach used to identify the location of the maximum ground-level concentration is very fast (less than 3 or 4 iterations).

The recommendation to change the calculation of buoyancy flux F is a good one (see Equation (2.4)). It would be more convenient and more standard for the user to input the ambient air temperature and stack gas temperature needed for this equation rather than the enthalpy and stack gas density that are presently needed. We will make this change upon approval.

H.E. Cramer Company, Inc. points out that σ_z(limit) --> 0 as H --> H_{lid} (Equation 2.5). In the TOX-SCREEN model, H can never exceed 450 meters (Turner, 1970). H_{lid} is usually much greater than this maximum for H. If it should ever happen that H --> H_{lid} in TOX-SCREEN, the program will print an error message and stop.

The statement is made that the guidance on the selection of Holzworth (1972) mixing heights is inappropriate. The class D stability category (daytime) is used in the air compartment of the TOX-SCREEN model. The Guideline on Air Quality Models (EPA, 1978 pages A5-A15) recommends the afternoon climatological value for this category. If class D (night) was used, then the average of morning and afternoon mixing should be used (see page A15, EPA, 1978) as recommended by H.E. Cramer Company, Inc.

No attempt has been made to check that mass continuity in the TOX-SCREEN model is conserved due to the difficulty in doing so. It is possible to simulate three sources (one each to air, water and soil) simultaneously, in which case, the amount volatilized or resuspended to the air could be greater than that deposited. This was a concern stated in the review. While it is recognized that mass continuity is important, checking it in a screening type model such as TOX-SCREEN would be difficult if not impossible.

In conclusion, we feel that H.E. Cramer Company, Inc. have made some good suggestions in their review. However, it should be remembered that TOX-SCREEN is a screening-level model and should be viewed as such.

2.3 PREVIOUS TESTING RESULTS

2.3.1 Comparison with Measured Data

Preliminary testing of the TOX-SCREEN atmospheric model was performed by Oak Ridge Laboratory (Hetrick and McDowell-Boyer, informal report). The tests involved comparing simulated results for trichloroethylene (TCE) with observed concentrations downwind of a number of manufacturing plants in Texas and Louisiana, and near a site in West Virginia. The results are summarized below.

Comparisons were made for five sites: four point sources, and an area source. For each site, source emission rates and measured air concentrations were available. For the point sources, stack heights were assumed. Table 2.1 presents the important input common to the point source runs, and Table 2.2 presents the specific input and the results for all five sites.

TABLE 2.1 INPUT PARAMETERS FOR PREVIOUS AIR MODEL TESTS (From Hetrick and McDowell-Boyer, informal report)

Parameter	Definition	Value
UDG	Dry deposition velocity	0.01 m/s
WRATG	Washout ratio	2.27
AK	Degradation rate of chemical in air	1.6E-5 /s
HMIX	Mixing height	2.E3 m
HS	Stack height	50 m
VG	Gravitational settling velocity	0. m/s
VS	Stack gas exit velocity	0. m/s
SRAD	Stack radius	10. m
RHO	Stack gas density	6.6E-1 kg/m3
ENTPY	Stack gas enthalpy	2.5E5 J/kg
XLENS	Length of plume over soil	2.0E3 m

TABLE 2.2 INPUT PARAMETERS AND RESULTS OF PREVIOUS AIR MODEL TESTS (From Hetrick and McDowell-Boyer, informal report)

	Site				
	1	2	3	4	5
Input					
UW (wind speed - m/s)	8.	4.	4.	8.	7.
QS (source - kg/s)	2.7E-3	9.2E-3	9.1E-3	2.9E-3	2.E-3
CTYLTH (length of area - m)	-	-	-	-	1.E4
Results (Conc. (ug/m^3))					
Simulated (max)	16.2	117.	115.	17.6	-
Simulated (ave)	6.4	49.5	48.8	7.	0.675
Measured (ave)	14.6	442.	24.3	20.	-
Measured (range)	5.4- 62.	113.- 756.	10.3- 38.9	5.4- 81.	trace- 0.360

At three out of four point source sites, the calculated average concentrations were within a factor of three of the average measured values. Also, concentrations at three of the four sites were underpredicted; Hetrick and McDowell-Boyer (informal report) concluded that their assumed stack height may have caused the highly underpredicted value at Site 2.

2.3.2 Comparison with ATM

Further testing of the TOX-SCREEN atmospheric dispersion model was performed by Hetrick (1983a). In this test, TOX-SCREEN results were compared with the detailed atmospheric pollutant dispersion/deposition model ATM (Culkowski and Patterson, 1976). The three chemicals tested were methylene chloride, trichloroethylene (TCE), and a hypothetical compound for which a database of chemical characteristics is available in the U.S. EPA Office of Toxic Substances Graphical Exposure Modeling System (GEMS) (GSC, 1982).

TOX-SCREEN input data such as chemical characteristics, stack parameters, and source loading rates were derived from ATM input data. Since TOX-SCREEN uses monthly average wind speeds and a single wind direction, these data were obtained from averaged NOAA weather data for the same site as the STability ARray (STAR) data used in the ATM modeling effort. For each chemical, two TOX-SCREEN runs were made to determine the effect of varying the length of the plume over soil.

For comparison purposes, TOX-SCREEN monthly concentrations (both average and maximum) were averaged for a one year period. Since ATM calculates concentrations in several sectors in each of sixteen different directions, the TOX-SCREEN results were compared with averages of the sector concentrations in a particular direction, or maximum concentrations in a particular direction. The chosen direction was either that of the maximum or minimum calculated concentration.

The TOX-SCREEN results were much higher (factors of 10-63) than the corresponding ATM results for all chemicals except the hypothetical compound. For a plume length of 50 km, the models predicted similar concentrations for this chemical. Generally, Hetrick (1983a) concluded that the results were "reasonable"..."considering the differences between the two models."

2.4 SENSITIVITY TESTING

Based on the recommendation of H.E. Cramer Co. (HEC, 1983), we performed sensitivity analyses on several parameters used in the atmospheric model. Two sets of tests were performed:

1) The effects of deposition velocities and washout ratios on net deposition to soil/water surfaces were investigated; these tests are described in Section 5 (Intermedia Transfer).

2) The effects of pollutant point source characteristics (stack parameters, exit gas properties, etc) on pollutant concentrations in air were investigated; these tests are described below.

The input parameters varied in these tests were the mixing height, stack physical parameters (height and radius), and stack gas parameters (exit velocity, and gravitational settling velocity). Tests of the effects of stack gas enthalpy and density were also performed even though these parameters will likely be eliminated in a future version of TOX-SCREEN (ORNL, 1983). The intent of these tests was to discover any biases caused by inappropriate selection of 'difficult-to-determine' parameters. They are intended to show the relative sensitivity of TOX-SCREEN results to these parameters over ranges which encompass all likely values. This can indicate which parameters should receive more effort in data collection under similar application scenarios. Of course, the reader should note that other scenarios will modify the relative sensitivities of these parameters to some extent.

The base scenario for the tests was intentionally simple. The effects of pollutant degradation and intermedia transfer processes such as deposition and volatilization were eliminated, and wind speed and pollutant loading were kept constant. Typical or reasonable values for all parameters except the "test" parameters were used. The important input parameters used in the tests are shown in Table 2.3, where the seven test parameters are indicated by a "*". During each test sequence, the six remaining test parameters were kept constant at the values shown in Table 2.3, while the test parameter took on the values shown in Table 2.4. Thus, all sensitivity sequences are directly comparable.

The results of the tests are shown in Figures 2.1 - 2.7, where the concentration axes are identical to facilitate comparisons between parameters. Both the sector-averaged concentration

TABLE 2.3 INPUT PARAMETERS FOR AIR MODEL SENSITIVITY TESTS

Parameter	Definition	Value
AIRFLG	Signifies point source	POIN
AIRPOL	Signifies gaseous pollutant	GAS
QS	Pollutant source rate	0.001 kg/s
UW	Wind speed	3.0 m/s
UDG	Dry deposition velocity	0.0 m/s
WRATG	Washout ratio	0.0
AK	Degradation rate of chemical in air	0.0 /s
XLENS	Length of plume over soil	1.0E4 m
CUM	Initial pollutant in soil	0.0
HMIX *	Mixing height	2000. m
HS *	Stack height	75. m
SRAD *	Stack radius	3. m
VG *	Gravitational settling velocity	0.001 m/s
VS *	Stack gas exit velocity	1.0 m/s
RHO *	Stack gas density	0.75 kg/m3
ENTPY *	Stack gas enthalpy	1.0E4 J/kg

* signifies a test parameter

TABLE 2.4 VALUES OF TEST PARAMETERS FOR AIR MODEL SENSITIVITY ANALYSIS

HMIX (m)	200.	250.	500.	1000.	5000.		
HS (m)	10.	25.	50.	75.	100.	150.	200.
SRAD (m)	0.05	0.1	0.5	1.0	3.0	5.0	10.
VG (m/s)	.0001	.001	.005	0.01	0.05	0.1	0.5
VS (m/s)	0.1	0.5	1.0	5.0	10.	20.	
RHO(kg/m3)	0.25	0.5	0.75	1.0	1.5	2.0	
ENTPY (J/kg)	5.E3	1.E4	5.E4	1.E5	5.E5	7.5E5	

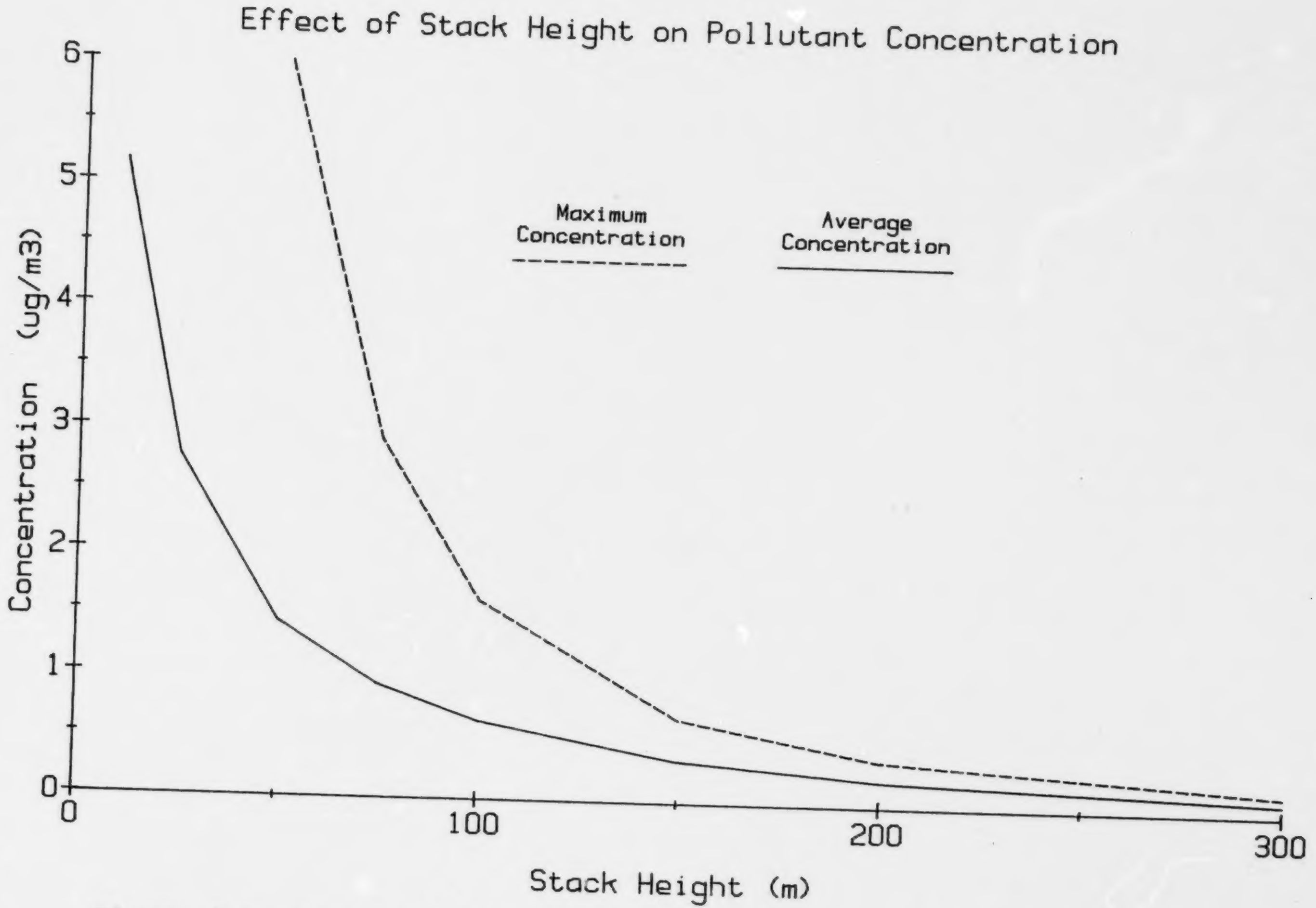

Figure 2.1 Sensitivity of air pollutant concentrations to stack height.

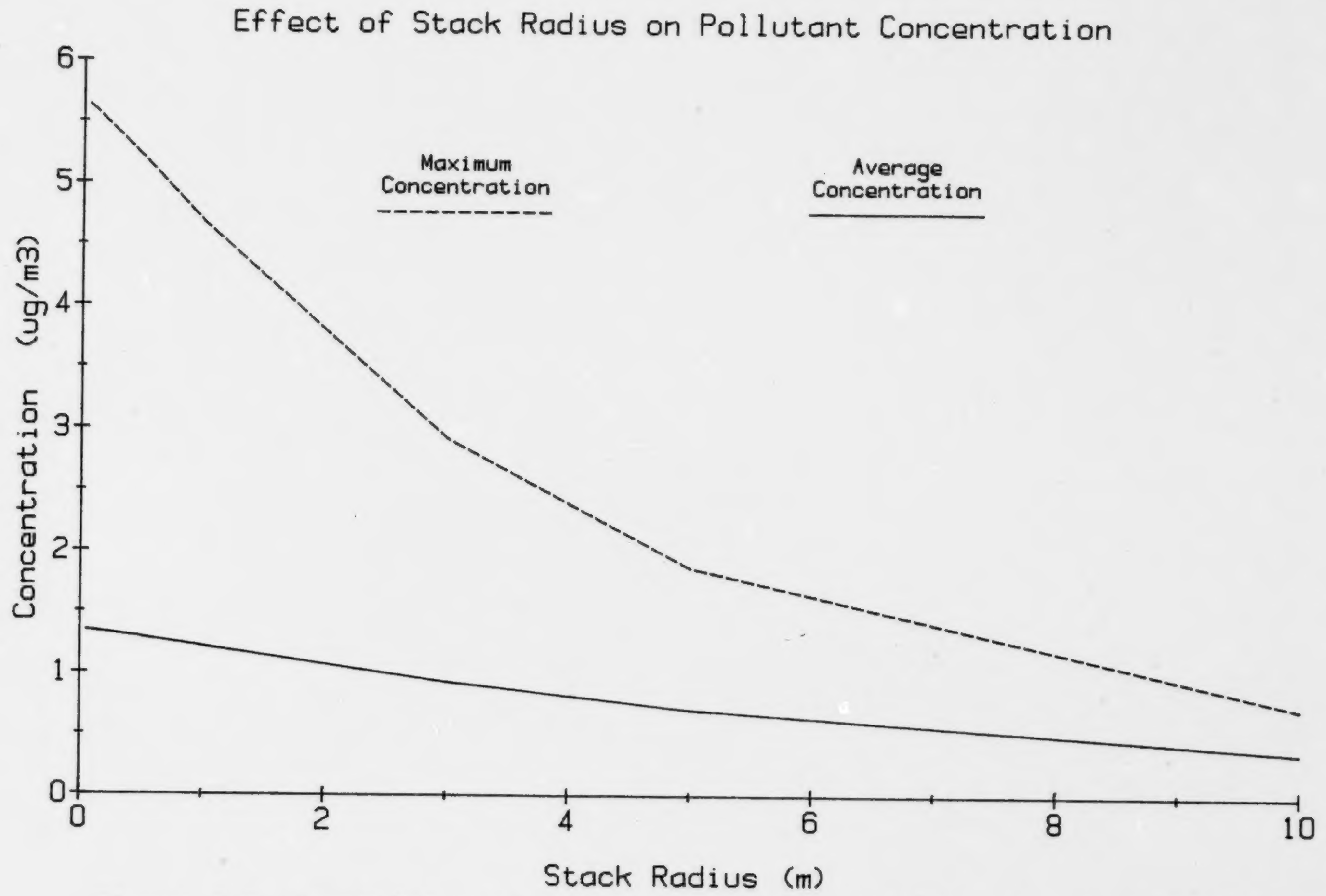

Figure 2.2 Sensitivity of air pollutant concentrations to stack radius.

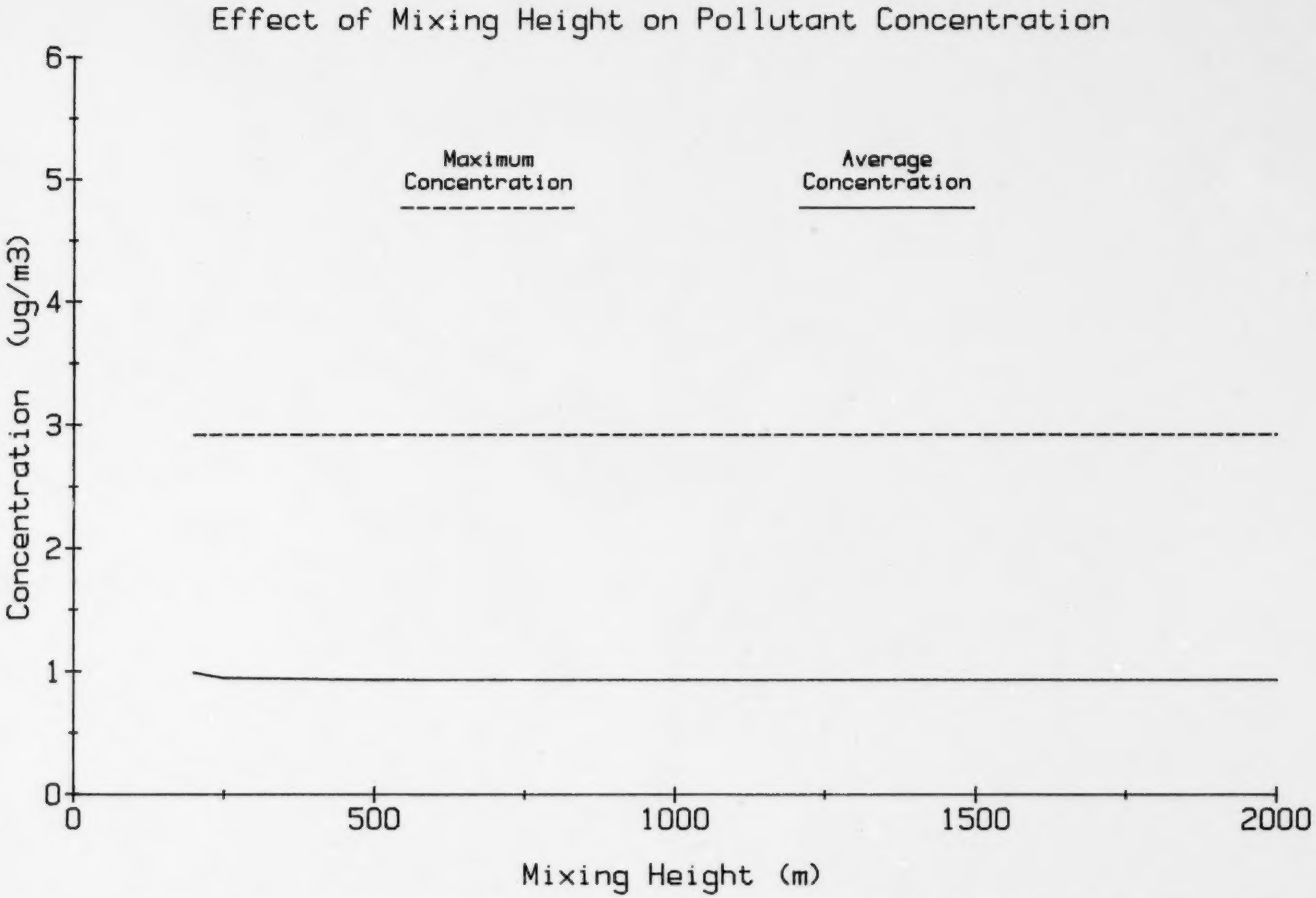

Figure 2.3 Sensitivity of air pollutant concentrations to mixing height.

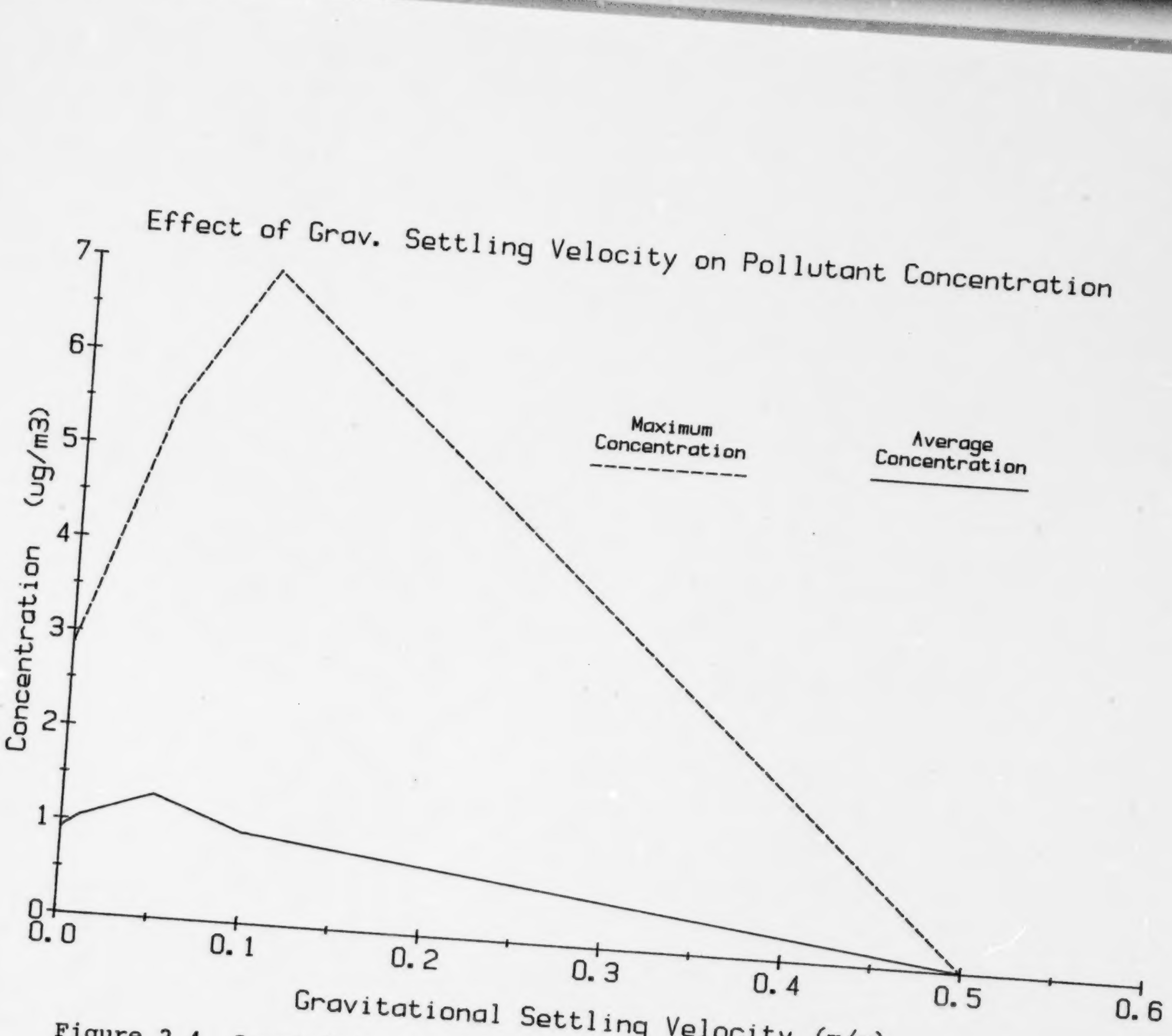

Figure 2.4 Sensitivity of air pollutant concentrations to gravitational settling velocity.

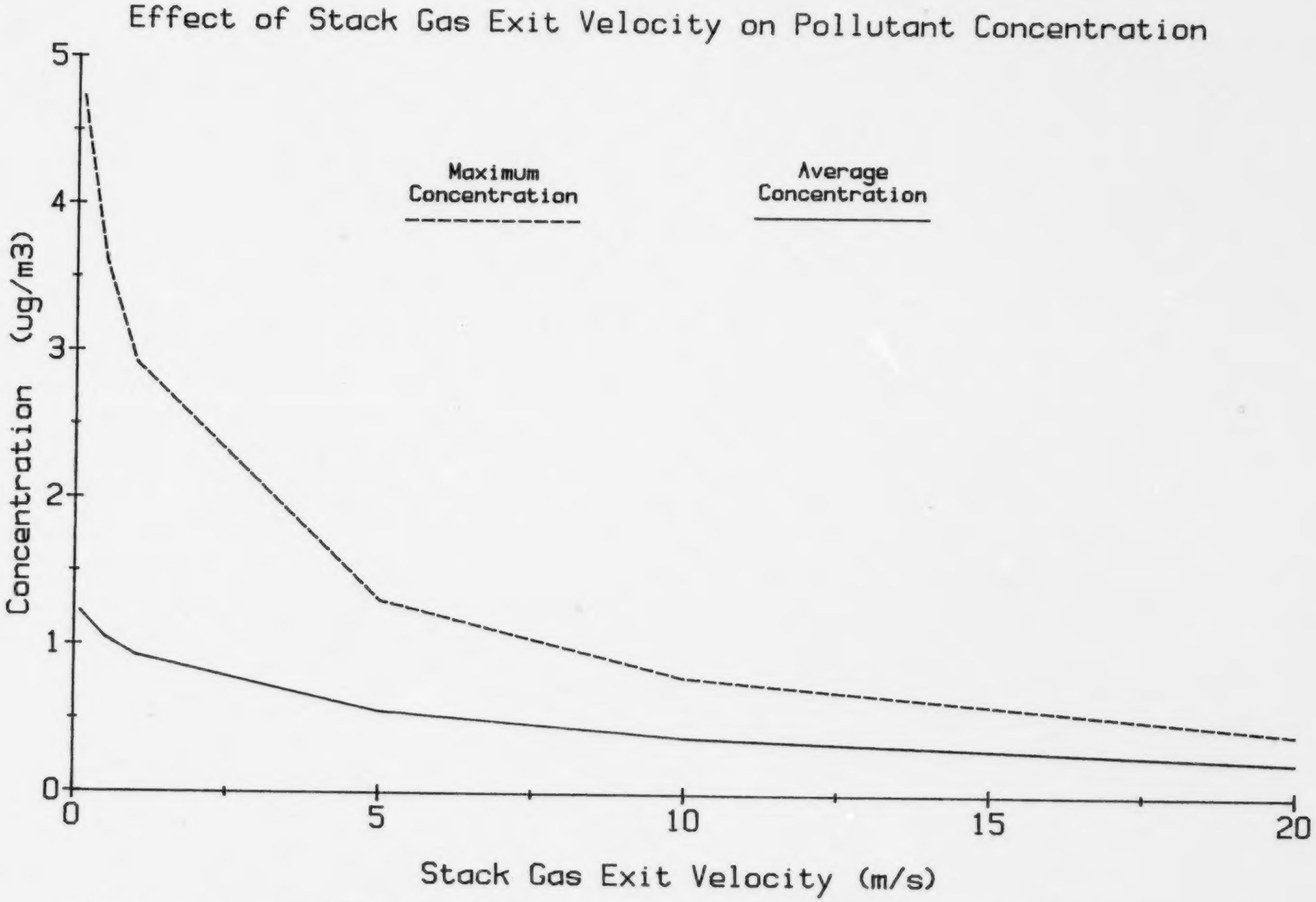

Figure 2.5 Sensitivity of air pollutant concentrations to stack gas exit velocity.

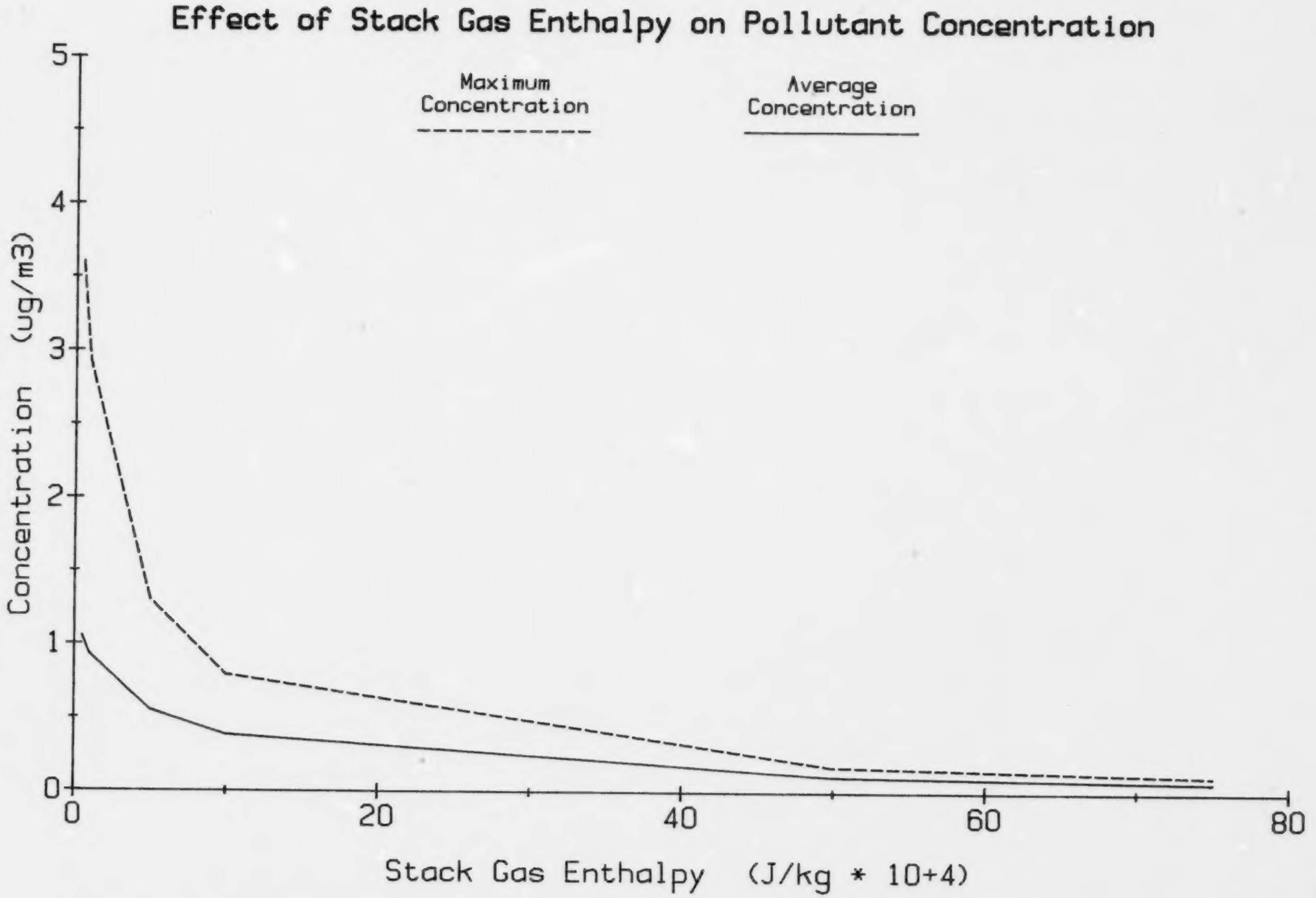

Figure 2.6 Sensitivity of air pollutant concentrations to stack gas enthalpy.

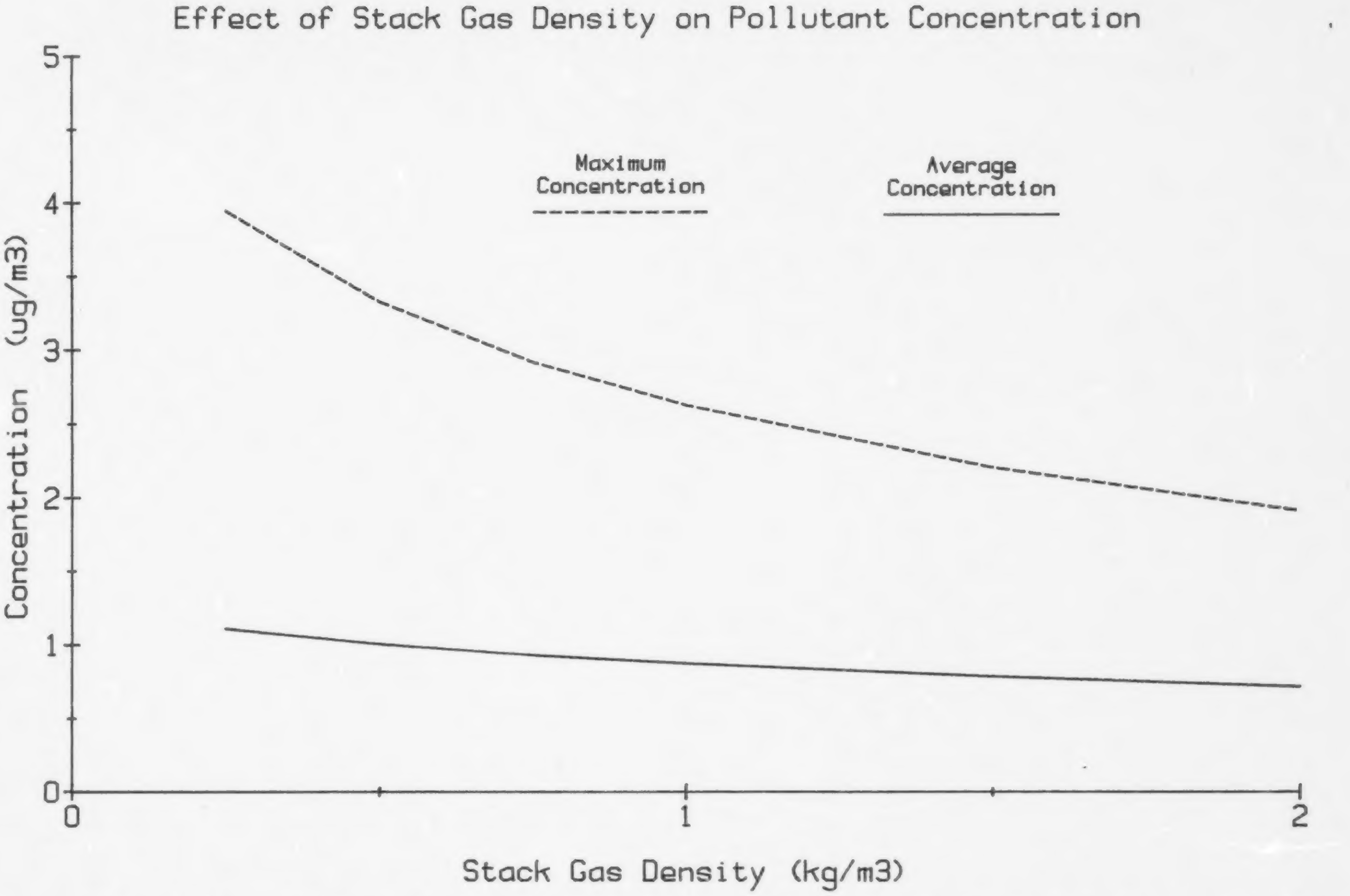

Figure 2.7 Sensitivity of air pollutant concentrations to stack gas density.

between X_{max} and X_{final} (see Section 5.1.2) and the maximum concentration (at X_{max}) are shown.

Under the base scenario selected, the determination of stack height appears most crucial to calculation of both average and maximum concentration. Also, maximum concentration is sensitive to stack radius, gravitational settling velocity, stack gas exit velocity, and stack gas enthalpy.

Since the concentration is inversely related to the effective stack height, which varies as direct functions of the stack height, radius, gas exit velocity, gas enthalpy, and gas density (see Eqns. 2-5 to 2-9 in MBH), the trends exhibited in these tests appear correct. However, these tests also suggest that confidence in the concentrations predicted by the TOX-SCREEN air model would be improved by the execution of a short sequence of sensitivity tests to ensure that the specific application scenario is relatively insensitive to uncertain parameters or to determine the range of uncertainty in results.

2.5 CONCLUSIONS

Based on a detailed review of the model by H. E. Cramer and analysis of previous and current testing results, the atmospheric dispersion model is appropriate to screen chemicals, with some reservations. These reservations are related to: 1) the inherent difficulties associated with simulating atmospheric pollutant concentrations caused by wide temporal and spatial variability in the environmental driving forces (wind direction and speed, precipitation, topography, air density/temperature stratification, etc.); 2) the sensitivity of model results to parameter estimates; and 3) the problem of checking mass continuity in this methodology, i.e. confirmation that intramedia and intermedia mass transfers are computed "correctly." Sensitivity to model parameters is problematic if the parameter values are uncertain. The model documentation should provide estimates of parameter uncertainties. Resolution of item 3 (mass conservation) is made more difficult by incorporation of an air model. The total mass in all media will not equal the mass emitted, since wind carries pollutants out of the model domain. However, a reasonable mass balance test could be incorporated in the program, and would be worth the effort.

In their review of the air model, H. E. Cramer Co. (1983) discussed several issues which needed to be addressed. These issues, testing conclusions, and the reservations mentioned above, are discussed briefly in this section. The evaluation of atmospheric deposition is discussed in Section 5.

H. E. Cramer Co. recommends the replacement of the distance-dependent plume rise equations in order to simplify the model, eliminate an iterative technique, and increase the accuracy. ORNL (1983) suggest that while the recommended method is simpler, the relative accuracy of the two methods is uncertain, and the iterative technique is fast.

H. E. Cramer Co. recommends the replacement of the buoyancy flux (F) calculation in order to simplify the user input, and utilize a more standard and accepted method. ORNL agrees with the recommendation. The change will eliminate the stack gas density and enthalpy from the required input.

H. E. Cramer Co. recommends incorporation of a method to allow a pollutant plume which stabilizes near the top of the surface mixing layer to mix to the surface. ORNL suggests that the conditions described by H. E. Cramer Co. are rare, and if they occur TOX-SCREEN prints an error message and stops execution.

H. E. Cramer Co. recommends changing the recommended mixing height from "mean annual afternoon" to "average of mean annual early morning and afternoon" in order to eliminate a bias toward underestimation of ground-level concentrations at long downwind distances. ORNL cites EPA (1978) which recommends the "afternoon" mixing height for class D stability category (daytime), which is used in TOX-SCREEN.

We feel that ORNL has responded appropriately to the issues discussed above in light of the fact that TOX-SCREEN is a screening level model, and that the air model, while subject to large environmental uncertainties, is essentially a "....simplified version of current state-of-the art Gaussian dispersion models."

Analysis of the testing results presented in Sections 2.3 and 2.4 indicates that TOX-SCREEN air concentration predictions will not likely satisfy the expected "screening-level" accuracy of one order-of-magnitude (EPA, 1982). This is due to (1) the variability in factors which determine pollutant dispersion in air combined with the necessary simplicity of the model; (2) sensitivity to input parameters such as stack height and radius; and (3) the deliberate incorporation of conservatism such as constant wind direction. These last two effects are observed in the testing efforts described above. For example (1) McDowell-Boyer and Hetrick (informal report) conclude that incorrect stack height may have caused differences between observed and predicted results; (2) stack height is a relatively sensitive parameter (Section 2.4); and (3) comparison with ATM resulted in overpredictions by factors of 10 to 63 (Hetrick, 1983a). Because of the sensitivity of TOX-SCREEN air model to stack height, we recommend that either the documentation should provide guidance to the user on performing brief sensitivity testing to bracket the prediction, or alternately, modify the program to allow inputting a range for this (or other) parameters and calculation of a range of predicted concentrations.

SECTION 3

SOIL MODEL

3.1 REVIEW AND EVALUATION

The soil model incorporated in TOX-SCREEN is the SESOIL Model (Bonazountas and Wagner, 1981). The review and testing results presented in this section are preliminary, and are derived largely from work performed by Anderson-Nichols as part of a separate detailed evaluation of the stand-alone version of SESOIL (Watson and Brown, 1984).

3.1.1 Overview of SESOIL

SESOIL is an environmental assessment model designed by Arthur D. Little, Inc. to become: (1) a watershed model, (2) an unsaturated soil zone model, and (3) a ground-water model. SESOIL in its present form is only an unsaturated soil zone model. SESOIL calculates a seasonal water balance for a soil column extending from the land surface to the upper saturated soil zone (capillary fringe included). This water balance is then used to simulate pollutant transport.

SESOIL is the acronym for the SEasonal SOIL compartment model. SESOIL is designated "seasonal" because it statistically estimates the pollutant distribution in the soil column after a season (e.g., year or month) "directly". It does not estimate the pollutant distribution "indirectly" by summing pollutant distributions after each major storm event. Pollutant transport models can generally be classified as either deterministic models or stochastic models. At present, most of the models are deterministic. SESOIL is unique in that it uses a stochastic approach for the hydrologic cycle and a deterministic approach for pollutant transport. Also, SESOIL's stochastic approach (described below) is different from that of other stochastic models. It does not simply relate watershed response to precipitation based on analysis of historical data.

3.1.2 SESOIL Processes

The processes considered by SESOIL can be divided into three major groups: 1) hydrologic, 2) sediment erosion and 3) pollutant transport. The individual processes considered in each group are listed in Table 3.1.

Hydrologic Processes. The hydrologic process cycle drives the pollutant and sediment cycles, and is, therefore, the most important cycle.

The hydrologic cycle in SESOIL is based on a statistical dynamic formulation of the vertical water budget at the land-atmosphere interface (Eagleson, 1978). Physically based dynamic and conservation equations express the infiltration, exfiltration, transpiration, percolation to ground water, and capillary rise from the water table during and between storms in terms of the following independent variables: precipitation, potential evapotranspiration, soil properties, and water table elevation. Uncertainty is introduced into the hydrologic simulation equations via probability density functions of the independent climatic variables, producing derived probability distributions of the dependent water balance elements: surface runoff, evapotranspiration, and ground-water runoff. The mean values of these quantities give a long-term (seasonal) average water balance.

Intrinsic to Eagelson's analysis is the assumption that moisture storage over a "season" (year) does not change. Bonazountas and Wagner (1981) state that this assumption is most valid in arid to semi-arid climates where soil moisture content will reach an annual minimum during the dry season.

Although Eagelson (1978) derived his equations using a time step of one year, SESOIL employs both a yearly and monthly time step. To account for a change in moisture storage from month to month, SESOIL uses a change in moisture storage term for the entire soil column:

$$\Delta So = z\, n(So(t) - So(t-1)) \qquad (3.1)$$

TABLE 3.1 PROCESSES SIMULATED BY THE TOX-SCREEN VERSION OF SESOIL

Hydrologic

precipitation

infiltration/exfiltration

soil moisture

evapotranspiration

capillary rise

ground-water runoff

surface runoff

Sediment Erosion

resuspension by wind

erosion by water

Pollutant Transport

advection

diffusion/volatilization

degradation

adsorption

hydrolysis

cation exchange

complexation chemistry

where S_o = average seasonal soil saturation
z = length of soil column
t = time
n = porosity
ΔS_o = change in moisture storage

SESOIL uses a first-order water conservation equation and ten supplementary relations to solve for the average annual soil moisture (So). Based upon the dependent variable, So, any desired seasonal water balance component can be obtained. There are 21 unknowns in the water conservation and supplementary equations; 10 hydrologic parameters are input into SESOIL. Therefore, a combination of 11 unknowns and 11 equations are solved by SESOIL. Individual processes in the hydrologic cycle are simulated as follows:

> Seasonal precipitation - represented by rectangular pulses (Poisson arrivals) of random depth and duration based on the total precipitation, number of storms, and length of the rainy season.
>
> Infiltration/exfiltration - described by the Philip (1969) equation; assumes soil moisture before each storm and interstorm period is uniform at its long-term average.
>
> Percolation to ground water - steady throughout the rainy season and at a rate determined by the long-term average seasonal soil moisture; occurs only during the rainy season.
>
> Capillary rise - steady throughout the rainy season and at a rate determined by the long term average seasonal soil moisture; occurs only during the rainy season.
>
> Evapotranspiration - depends on soil, climate, storm sequence, and average rate of derived PET; PET solved by the Penman (1948) equation and ET solved by the Van den Honert (1948) equation.
>
> Surface runoff - derived from the distribution of rainstorm intensity and duration, and the calculated infiltration component.

In addition to the processes listed above, some other hydrologic factors are considered as follows:

Soil properties - determined by the method of Brooks and Corey (1966), unsaturated hydraulic conductivity is dependent on soil moisture content and the soil disconnectedness index.

Vertical soil heterogeneity - layering is considered by taking the weighted mean of the saturated hydraulic conductivity of the soil layers or:

$$K_z = \frac{d}{\sum_{i=1}^{n} \frac{d_i}{K_i}} \qquad (3.2)$$

where K_z = vertically averaged hydraulic conductivity
K_i = hydraulic conductivity of each layer
d = total thickness
d_i = thickness of each layer

Sediment Erosion Processes. The stand-alone version of SESOIL does not simulate the processes of sediment erosion by water or sediment resuspension by wind. However, the effect of these soil loss processes on pollutant transport are estimated by empirical equations incorporated in the TOX-SCREEN program. These equations are discussed in Section 5 (Intermedia Transfer).

Pollutant Transport Processes. The pollutant cycle employed by SESOIL is intricately involved and controlled by the hydrologic cycle. SESOIL uses a mass balance concept in modeling pollutant concentrations: a) on the soil matrix, b) in the soil moisture, and c) in the soil air (gaseous phase).

The pollutant cycle accounts for more than 12 chemical processes. Some alternative simulation options are available.

Diffusion/Volatilization - described by Fick's first law; estimates upward mass flow in the soil column to the air as volatilization; assumes pollutant buried under layer of clean soil, and vapor phase diffusion is rate controlling. The Farmer et al. (1980) model is used in SESOIL (see Section 5).

Adsorption/desorption - represented by Freundlich isotherm.

Degradation - first-order decay.

Hydrolysis - allows neutral and acid or base catalyzed hydrolysis; assumes first-order decay.

Cation exchange - irreversible, instantaneous process which immobilizes pollutant up to the soil cation exchange capacity.

Complexation chemistry - metal ion in solution is complexed by organic ligand(s) resulting in a soluble compound; assumed to be an equilibrium process.

The depth to which the pollutant has traveled is defined in SESOIL as the average of the infiltration rate and the ground-water recharge rate divided by the product of the porosity and the moisture content (see pages PT-57 and 58 in Bonazountas and Wagner, 1981). According to the model's developer, moisture content is defined in SESOIL as the ratio of the volume of water to the volume of voids, as opposed to the more traditional definition, i.e., ratio of the volume of water to the total volume (Bonazountas, 1984b). The user's manual, however, implies that the latter definition is used. Apparently, this inconsistency will be resolved in the new version of SESOIL by removing porosity from the relationship and by using the more traditional definition of moisture content (Bonazountas, 1984b).

SESOIL as implemented in TOX-SCREEN is designed to be used with 3 layers in the soil column, and apparently operates on a monthly basis. However, SESOIL pollutant cycle equations are written with an explicit time step. In TOX-SCREEN the equations are solved ten times per month to increase their accuracy (Hetrick and McDowell-Boyer, 1984). Each soil layer has its own mass balance pollutant equation and can release and receive pollutants from other layers.

3.1.3 Level of Effort Required for Data Input

The input data needed for executing SESOIL is fairly simple and staightforward compared to detailed soil compartment models; however, some effort may be required on the user's part to reduce the data to a suitable form for SESOIL. Data input can be divided into 4 groups: 1) climate data, 2) soil data, 3) chemical data, and 4) initial pollutant distribution in the soil column.

Climatic data acquisition takes the most time and effort in executing SESOIL. The recommended source of climatic input data are NOAA records. This data must be reduced for SESOIL usage. Monthly mean values of storm duration, depth of rain, number of storm events, temperature and other similar parameters must be calculated by hand or some other method. Acquiring this data can be time consuming, but less effort is required than for models which use time series input.

Soil input data is simple and straightforward, and consistent with being a screening model. The only parameter that might not be found in the literature is the soil disconnectedness index (C), however, SESOIL provides default values for all soil parameters including C. However, SESOIL default hydraulic conductivities should be used with caution because of inconsistencies.

Chemical input data to SESOIL should be available in chemical handbooks and the like, and initial pollutant distribution in the soil column can be defined by the user.

3.1.4 Comparison with Other Methods

Other models besides SESOIL that could be used for predicting chemical fate and movement in an unsaturated soil column include the analytical and numerical solutions to the 1-D convective-dispersive solute transport equation, and simplified versions of such computer models as PRZM (Carsel et al., 1982), HSPF (Johanson et al., 1981), and FEMWATER/FEMWASTE (Yeh and Ward, 1979, 1981). These models can be divided into: 1) physically based models which solve the continuity and flow equations, 2) water budget type models, and 3) a combination of 1) and 2).

The physically based models use the physically based continuity, mass transport, and Darcy's Law equations to derive the appropriate flow and solute transport equations. These equations can then be solved by analytical or numerical methods. FEMWATER/FEMWASTE is an example of a physically based model. Physically based models can require a large amount of detailed information that may be difficult to obtain. However, if enough detailed information is known the physically based models should provide the most accurate simulation results.

Water balance models use such concepts as PET, field capacity, and wilting point to compile daily water balances in several soil compartments. Water balance models have the advantage of needing limited data inputs but the disadvantage of being based on soil properties which are somewhat over-simplified. Also the budget models sometimes incorporate empirical relationships that may or may not be extended to other soil and climate conditions which the relationships were not derived for.

PRZM is a good example of a combination of the two types. It uses the water balance method to simulate the hydrology, while pollutant transport is computed by a numerical solution of the 1-D convective-dispersive solute transport equation.

The SESOIL model probably best fits into the water budget model category. Although SESOIL does not use the concepts of wilting point and field capacity it does use a water balance approach to solve for a monthly "average" infiltration and ground-water recharge rate. The soluble fraction of a pollutant is then moved downward at these rates. Data input is simple. SESOIL is at a disadvantage over other water budget models because it does not account for daily changes in moisture movement. SESOIL also uses several empirical relationships in solving for its' monthly water budget.

SESOIL can probably be considered less exact than other water budget models that consider daily rainfall (even though the other models use the concept of field capacity and wilting point) and definitely less exact than the physically based equations. The biggest advantage of SESOIL is that it is easily used, and limited data are needed to execute the model.

3.2 PREVIOUS TESTING RESULTS

Testing of the SESOIL model has been completed or is in the process of being completed by Arthur D. Little Inc.; Oak Ridge National Laboratory; Battelle, Pacific Northwest Laboratories; the EPA Environmental Monitoring and Surveillance Laboratory (EMSL), in Las Vegas, Nevada; and current efforts by Anderson-Nichols. Each testing effort by the other organizations is briefly described below, while preliminary testing results by Anderson-Nichols are discussed in Section 3.3.

3.2.1 Testing by Arthur D. Little, Inc.

Arthur D. Little has completed two testing efforts. The first was an application/validation study conducted on two field sites, one in Kansas and one in Montana (Bonazountas et al., 1982). Field data and SESOIL simulations were compared for the metals chromium, copper, nickel, and sodium at the Kansas site and the organic compounds naphthalene and anthracene at the Montana site. SESOIL was calibrated by adjusting the adsorption coefficient and soil permeability. As shown in Table 3.2, concentrations of metals in the soil were consistently underestimated. The copper and nickel results were within 30% and 70% of the observed values, and Bonazountas et al. (1982) concluded that the differences were caused by uncertainty in input parameters and experimental data (observed values). They also suggested that the sodium differences were caused by the absence of clay swelling due to cation exchange effects, and an inappropriate adsorption coefficient.

At the Montana site, the concentrations of organic compounds were overestimated by SESOIL by factors of 5 and 2.3 (see Table 3.2). The differences were attributed to the lack of biodegradation rate data for the site (Bonazountas et al., 1982).

Sensitivity analyses were also conducted, as part of the first testing effort, on climatologic, soil, chemistry, and pollutant loading parameters. While these tests were of limited value in evaluating specific model capabilities, they indicated that the model was not overly sensitive to the parameter ranges tested. It should be noted that the SESOIL version tested in these applications considered only two soil layers while the TOX-SCREEN version considers three layers.

The second testing effort conducted by Arthur D. Little was a study of the fate of 6 pollutants in 3 climates with 4 soil types (Wagner et al., 1983). Volatilization and adsorption were taken to be the primary chemical processes. Freon, TCE, methylene chloride, methylchloroform, perchloroethylene, and carbon tetrachloride were the pollutants selected for analysis. The majority of this testing effort was devoted to analyzing the sensitivity of the SESOIL volatilization and adsorption routines to climate, soil type, depth of soil covering layer, depth to ground water, and soil heterogeneity. Hydrologic cycle comparisons such as changes in ground-water recharge with changes in soil type and variation of moisture content with soil type and ground-water recharge were also investigated. There was no comparison of SESOIL results to field data in this effort. The principal conclusion regarding the model was that volatilization was overestimated, partially because this process is allowed to occur from any soil depth (Wagner et al., 1983).

TABLE 3.2 COMPARISON OF SESOIL PREDICTIONS WITH MEASURED POLLUTANT CONCENTRATIONS AT TWO LAND TREATMENT SITES (Bonazountas et al., 1982)

SITE 1 - METALS (mg/l)

	SESOIL (1)	OBSERVED (2)
Chromium		
Upper Layer	0.147	0.80
Lower Layer	0.0	1.00
Copper		
Upper Layer	0.136	0.20
Lower Layer	8.1E-5	0.00
Nickel		
Upper Layer	0.0582	0.20
Lower Layer	1.95E-4	0.00
Sodium		
Upper Layer	0.0	89.
Lower Layer	1.9	114.

SITE 2 - ORGANIC CHEMICALS (mg/l)

	SESOIL (3)	OBSERVED (2)
Naphthalene		
Upper Layer	18.3	3.69
Lower Layer	.00312	-
Anthracene		
Upper Layer	5.55	2.36
Lower Layer	4.81E-5	-

(1) Upper Layer: 0-15 cm; Lower Layer: 15-5000 cm

(2) Upper Layer: 0-15 cm; Lower Layer: 15-30 cm

(3) Upper Layer: 0-20 cm; Lower Layer: 20-5000 cm

3.2.2 Testing by Oak Ridge National Laboratory

SESOIL was compared with the hydrologic model AGTEHM (Hetrick et al., 1982), for two different field sites, one in Arkansas and one in South Carolina (Hetrick, 1983b). AGTEHM is a detailed mechanistic model of hydrology in a vegetative/soil system. It uses hourly rainfall and other climatic data along with soil hydraulic properties to simulate the water balance, on an hourly basis, through a layered biotic and soil column. SESOIL output was calibrated to AGTEHM results via the pore disconnectedness parameter (C). Only SESOIL hydrologic cycle components were calibrated and compared to AGTEHM simulations. An increase in C caused an increase in soil moisture, no change in infiltration, an increase in evapotranspiration, and a decrease in ground-water runoff.

From the results reviewed, it was apparent that SESOIL could be adequately calibrated to AGTEHM results using C. For the Arkansas site, monthly values of soil moisture, infiltration, and surface runoff predicted by the two models never varied by more than a factor of 2. Evapotranspiration and ground-water runoff differences were less than a factor of 7. However, it was also apparent that SESOIL results are very sensitive to the C parameter.

3.2.3 Testing by Battelle, Pacific Northwest Laboratories

Battelle recently completed a study involving the comparison of a number of flow, transport and geochemical models for soil and ground-water systems. SESOIL was one of those tested. Battelle designed a detailed landfill test problem for use in comparing unsaturated zone model predictions. The test problem was primarily directed at water movement, rather than pollutant transport. Kincaid et al. (1984) concluded that because SESOIL characterizes the soil column as homogeneous for purposes of solving the water balance, the model was not useful for analyzing sites exhibiting a high degree of layering. This limitation was particularly evident when SESOIL results for the landfill test case were compared with those of other models tested. Kincaid et al. (1984) suggest that SESOIL is best suited for screening analyses and coarse long-term assessments.

3.2.4 Testing by EPA-EMSL

EPA-EMSL will be comparing solute transport data from laboratory soil columns 1-2 meters in height to pollutant transport model results. Four organic compounds will be selected for the comparison study. SESOIL will be one of the models tested. EPA-EMSL is in the process of screening the chemicals that will be used in the soil column experiments. Actual testing results will become available in late 1984.

3.3 CURRENT TESTING RESULTS

Anderson-Nichols has completed testing of the "stand-alone" version of SESOIL (Watson and Brown, 1984). The testing procedure involved comparing SESOIL results to both simple analytical solutions of the one-dimensional, convection-dispersion solute transport equation, and field data from sites in Florida, Georgia and Wisconsin. As part of this testing, calculational errors in SESOIL were discovered which affect the maximum depth of pollutant penetration in the soil column. The errors were corrected in the test version; consequently, the preliminary results and conclusions discussed below are based on a recent and more correct version of SESOIL than that incorporated in TOX-SCREEN. It is assumed that these corrections will also be implemented in TOX-SCREEN.

The reader is referred to Watson and Brown (1984) for details of the testing procedures and results. The following are a series of conclusions based on their testing of SESOIL:

1. The basic framework for a useful, screening level, chemical migration and fate model exists in SESOIL. The model is relatively easy to use, input data are easy to compile, and most of the model parameters can be readily estimated. Key processes are simulated at an appropriate level of sophistication for a screening tool. In particular, the hydrologic cycle appears to be sound, with the exception of an error in the evapotranspiration algorithm. There are several errors in the pollutant cycle that require correction and several modifications that should be considered. Errors exist in the neutral hydrolysis and depth of pollutant penetration algorithms. Modifications recommended for consideration include relating the depth of pollutant penetration to the sorptive properties of the chemical and the replacement of the runoff participation factor with a

more process-oriented description of chemical washoff from the land surface.

2. SESOIL can be applied to generic environmental conditions for purposes of evaluating the relative behavior of different chemicals, if model limitations are kept in mind and judgement is used in the estimation of model parameters. Site-specific applications require model calibration.

3. SESOIL cannot be applied to sites exhibiting large vertical variations in soil properties.

4. Consideration should be given to modifying the algorithm used to determine when chemical will begin to leach to ground water. This algorithm is based only on the estimated travel time for water; the sorptive properties of the chemical are not considered. Thus, for a given environmental setting, all chemicals will initially reach ground water at the same time.

5. The SESOIL documentation report/user's manual provides an extensive review of the literature in many areas. While this review is useful at times, it also serves to confuse the user. The documentation is not explicit in terms of the specific processes that are considered and the theory that is incorporated in the model. The documentation is also not explicit in terms of parameter estimation. The parameter estimation guidance is often confusing and, in some cases, incorrect.

6. The applicability of the model is more limited than the developers suggest. There are limitations associated with using SESOIL as a watershed model, particularly with respect to predicting runoff losses. There are limitations associated with applying SESOIL to certain disposal facilities (e.g., landfills) where large variations in soil properties may cause the hydrologic cycle algorithms to break down. Application of SESOIL to certain release scenarios (e.g., spills, buried drums and tank leaks) is also limited because of the limitations in the volatilization and soil diffusion algorithms.

SECTION 4

AQUATIC MODELS

The aquatic models were evaluated similarly to the air and soil models. First the individual models (river, lake, estuary, and ocean outfall) were reviewed and compared with other aquatic pollutant fate and transport models, and the important assumptions, advantages, and deficiencies of TOX-SCREEN methods were discussed. Second, TOX-SCREEN testing work performed elsewhere was reviewed, and selected results presented. Third, the TOX-SCREEN river, lake, and estuary models were tested by comparison with observed pollutant concentrations and other model predictions.

4.1 REVIEW AND EVALUATION

The river, lake, estuary, and ocean models of the TOX-SCREEN model system were evaluated qualitatively against other analytical models designed for screening toxic chemicals. Such models include: Burns et al. (1982), Ditoro et al. (1981), Ditoro et al. (1982), Codell et al. (1982), Codell (1978), Johanson et al. (1982), Shull and Gloyna (1968), Shih and Gloyna (1970), Pritchard (1969), and Mills et al. (1982). This review is intended to determine how the models compare with other methods for simulating pollutant concentrations in water bodies; issues addressed include the important assumptions or deficiencies of the TOX-SCREEN models, their degree of conservatism, and their appropriateness for use in screening chemicals.

4.1.1 River Model

Model Description. The river and lake models use specified compartments or boxes to estimate mass balance or flux. Mass flux incorporates transformation and transport of a dissolved contaminant, and equilibrium partitioning for adsorbed species based on K_d. Uniform geometry between segments is required; up to 10 segments may be specified. Branching rivers or ones with multiple inflows and outflows cannot be represented accurately. Concentrations are calculated 10 times per month. Loading and stream velocity must be steady for each month. Mixing is assumed to be complete and instantaneous; dispersion is not accounted for because of the well-mixed compartment scheme. All transformation reactions are first-order, and affect the dissolved neutral species only. Acid/base reactions and adsorption are assumed to be at equilibrium. Suspended sediment concentrations can be input, or calculated using Laursens (1958) formula. A sediment bed is not represented.

Comparison With Other Models. TOX-SCREEN's mass flux equation for dissolved species is quite similar to other analytical compartment models. The mass flux equation is a simplification of the one in the U.S. EPA EXAMS model (Burns et al., 1982). Ditoro et al. (1981) employ mass flux equations for contaminant movement in both water column and sediment bed compartments.

Other analytical river models compute downstream concentrations according to time of travel to a specified point (Codell 1978, Shih and Gloyna 1970, Shull and Gloyna 1968). RIVLAK (Codell et al., 1982) is one of the few 2-dimensional transport analytical models. RIVLAK uses a vertical line source with x, y coordinates to compute the concentration at a given point downstream on a river or lake.

TOX-SCREEN calculates the homogeneous pollutant concentrations of dissolved neutral, dissolved ionic, and adsorbed forms in each reach. The equilibrium concentrations are based on an acid or base dissociation constant and a sediment-water partition coefficient. EXAMS also incorporates speciation in this manner. Transformation processes of photolysis, hydrolysis, oxidation, biodegradation, and volatilization are represented by first-order reactions. Only the undissociated dissolved fraction is subject to transformation, however. Simulation of these first-order processes is similar in other models. However, EXAMS accounts for variations in environmental conditions by modifying the transformation rates, and Ditoro et al. include a lumped decay coefficient summing all degradation processes in the sediment, also.

An interesting feature of the TOX-SCREEN river model is the incorporation of an algorithm to calculate suspended sediment concentrations. Many organic pollutants are hydrophobic, and are apt to be transported via suspended sediments. Only two other analytical river models reviewed calculate suspended sediment concentrations: Ditoro et al. (1981), and Shull and Gloyna (1968). Ditoro et al. utilize input settling and resuspension velocities of sediments. None of the models can simulate sediment transport; the average suspended sediment concentrations are calculated, then the contaminant is partitioned upon the mass flux into the compartment. The TOX-SCREEN models do not incorporate sediment bed-water column interactions; this is discussed in the next section.

Important Advantages/Deficiencies. The TOX-SCREEN model offers a number of advantages over other analytical screening models. The intermedia transfers such as wet-dry deposition from air to water, and soil to water transfers such as surface runoff, soil erosion (washload), and ground-water runoff allow for the evaluation of instream contamination from indirect sources. The relative positioning and size of media allows for a quantitative assessment of intermedia transport. Another advantage is the use of generic and simple parameters. The TOX-SCREEN documentation (McDowell-Boyer and Hetrick, 1982) provides canonical values for many aquatic model parameters, based on specific water bodies or regions.

The TOX-SCREEN river model has two major deficiencies:

1) it has no algorithm to account for sediment bed-water column interactions, such as diffusion and erosion/deposition, and

2) the suspended sediment calculation model is inappropriate for low flow conditions.

The absence of sediment bed-water column algorithms may not allow for an accurate representation of contaminant partitioning between the air, water, biota, and sediments. Other aquatic models account for the sediment bed as specific compartments. For example, in Ditoro et al. the mass balance equation for total chemical concentration in the sediment can be summarized as:

$$\frac{dC_{BED}}{dt} = \frac{dC_{BED}}{dt}\ \text{KINETIC} + \frac{dC_{BED}}{dt}\ \text{DIFFUSION} + \frac{dC_{BED}}{dt}\ \text{PARTICLE TRANSPORT} \tag{4.1}$$

Thus, transformation, diffusion of the dissolved contaminant between the water column and interstitial water, and erosion/deposition of contaminated sediments are simulated for pollutant mass flux between the sediment bed compartment and the overlying water column compartment. In addition, the loss of particulate sediment contaminants via burial is expressed in terms of a sedimentation velocity, which accounts for particles leaving the active sediment layer as sediment depth increases via sedimentation. For many chemicals, long-term evaluation of environmental partitioning requires the consideration of sediment bed-water column interactions.

The TOX-SCREEN river model can utilize input data for suspended sediments, or can calculate the average suspended sediment concentrations using Laursens (1958) formula. The contaminant is then partitioned using Kd assuming equilibrium as described above. Laursens formula is very sensitive to the boundary shear associated with sediment particles. Consequently, low in-stream velocities will not cause erosion of sediments. Because an average velocity is used for each month and uniform segment geometry is required, suspended sediment concentrations can vary temporally (monthly) but not spatially.

Laursen's formula computes boundary shear as:

$$\tau_o' = \frac{\gamma v^2}{590.0928} \left(\frac{d_i}{y_o}\right)^{1/3} \tag{4.2}$$

where τ_o' = boundary shear associated with sediment particles (kg/m^2)
γ = water density ($1000\ kg/m^3$)
V = water velocity (m/s)
d_i = median sediment particle diameter of size class i (m)
y_o = water depth (m)

The constant 540.028 (s^2/m) is provided in Laursen's paper (1958). The boundary shear is very sensitive to changes in velocity. The critical tractive force is expressed as:

$$\tau_c = \phi(\gamma_s - \gamma)\ d_i \tag{4.3}$$

where τ_c = critical tractive force (kg/m^2)
ϕ = Shields factor
γ_s = sediment density (kg/m^3)

The Shields factor represents the limit below which particles will not move. This factor and the sediment fall velocity are calculated in the program using a cubic spline, values of which were taken from a curve in Bagnold (1966), although the documentation states the parameter value may be obtained from curves provided in Appendix B. The Shields factor can prevent erosion if the sediment particle size is large; critical tractive force is then less than boundary shear, and suspended sediment calculations are stopped.

There are a number of predictive expressions available for calculating sediment bed material loading. The simplest is the Duboys relationship (Task Committee on Preparation of Sedimentation Manual, 1971). This expression is limited to uniform flow conditions in alluvial channels. Critical tractive force can be estimated using a nomograph with median size of the bed sediments, and the boundary shear can be derived from the hydraulic radius and slope of the channel. This technique will allow the calculation of suspended sediments for low in-stream velocities, although it and other techniques such as Yang (1976), are usually more accurate with high flow conditions. In general, Duboy tends to overpredict suspended sediment concentrations, while TOX-SCREEN (Laursen's formula) tends to underpredict these concentrations.

A minor (and easily corrected) problem in the code is that suspended sediment concentrations are not provided in the output. The adsorbed fraction of the pollutant is output, but there is no way to cross-check calculated suspended sediment concentrations with observed values.

All of TOX-SCREEN'S aquatic models calculate concentrations ten times per month, with end-of-month results printed. Average values for velocity and loading are used for each month, making the models unsuitable for simulation of pulse loading unless the duration of the pulse can be approximated by a monthly interval. Pollutant flux from contaminated soils (i.e., erosion and runoff) cannot be simulated for individual events. However, the current time resolution in TOX-SCREEN should be acceptable for a screening level model.

4.1.2 Lake Model

Model Description and Comparison With Other Models. The lake model utilizes the same pollutant processes and mass balance equation as does the river model, necessitating the assumption of complete and instantaneous mixing. The lake is considered as one compartment with an average velocity for flow out of the lake as stated in McDowell-Boyer and Hetrick (1982). Suspended sediment concentrations can be input or calculated using Laursens formula, which estimates concentration in the incoming stream to the lake. The in-lake suspended sediment concentrations are then calculated with a simple trapping efficiency algorithm, in which the efficiency is computed from a curve based on lake inflow and volume.

Ditoro et al. (1981) utilize the same compartment scheme for lakes, except sediment beds are included and are treated as separate compartments. Both inflow and outflow rates for the water column compartment are specified. The sediment bed compartment also incorporates kinetic transformation, diffusion, and sediment particle exchange rates between the bed and water column. RIVLAK (Codell et al., 1982) can simulate transport of a non-conservative contaminant along the near-shore region of a large lake from a non-steady source. RIVLAK requires a straight shoreline and steady flow. Concentrations are calculated for a specific point with x, y coordinates in time. The contaminant is released along a vertical line source and simulated for transport using a simplified two-dimensional advection/dispersion equation. This type of analysis is more applicable to near-field concentration estimates, and is useful for mixing zone criteria as well as for determining peak concentration.

The TOX-SCREEN lake model is more similar to the EXAMS model in terms of simulation of pollutant mass flux and acid/base speciation. However, TOX-SCREEN does not consider exchange processes between a sediment bed and the water column.

Important Advantages/Deficiencies. The lake model's advantages are the same as for the river model: intermedia loading of pollutants, and use of simple parameters.

A deficiency of the lake model is confusion about the solution to the mass transport equation. The documentation states that the velocity of water *out* of the lake must be specified in order to obtain a rate at which the pollutant is transported out of the lake. The total *rate* of loss of pollutant from the lake is computed in the code as a sum of degradation and advective rates as follows:

$$\mathrm{WKTL} = (\mathrm{WKTOT})\,(\mathrm{A1L}) + \mathrm{WKDL} \tag{4.4}$$

where WKTL = mass flux rate out of lake (/s)
WKTOT = sum of hydrolysis, biodegradation, oxidation, photolysis, and volatilization rates (/s)
A1L = undissociated dissolved fraction of the pollutant (-)

WKDL = rate at which water flows out of lake (/s)

The "flow" rate out of the lake (WKDL) is computed by the following equation:

$$WKDL = WVELL/(AREALK)^{1/2} \qquad (4.5)$$

where
WVELL = current velocity (m/s) for each month simulated
AREALK = surface area of lake (m^2)

The User's Manual (Hetrick and McDowell-Boyer, 1984) states that the user-specified velocity is the velocity out of the lake, implying the velocity of an outlet stream. However, as indicated in Eqn. 4.5, where a characteristic length of the lake is used, TOX-SCREEN assumes that this velocity is the velocity of the lake, which would generally be much less than the outlet stream or river. Thus the predicted inlake concentrations will be low due to a low hydraulic detention time (i.e., higher advection losses.) It should be noted that Appendix B of McDowell-Boyer and Hetrick (1982) lists the flow rate out of the lake (m^3/s) as a user-specified parameter, whereas actually, the velocity (m/s) is input. This contributes to the confusion discussed above. To avoid confusion, we recommend that the input parameter specifying velocity of lakes and rivers be changed to flow rate (m^3/s), or at least that the required input parameter be well defined.

Another deficiency is the lack of sediment bed-water column processes. These processes are more important in lakes, where dominant mass flux mechanisms are contaminant diffusion between the sediment bed and the water column, and the various transformation processes in each compartment, including bio-accumulation.

Since one option for determining the inlake suspended sediment concentration depends on the inflow suspended sediment concentration as computed by the Laursen (1958) method, the deficiency noted with this method and discussed in Section 4.1.1 is applicable to the lake model also.

4.1.3 Estuary Model

Model Description and Comparison With Other Models. The estuary model utilizes a one-dimensional steady-state advection/dispersion equation for transport of dissolved contaminants. The assumptions of the model include: average cross-sectional area; constant tidal and section-averaged, longitudinal dispersion coefficient; and a constant fresh water velocity. A maximum tidal velocity value may be substituted for the longitudinal dispersion coefficient. The estuary is broken into reaches with uniform geometry. Waste loading is assumed to be in the center of the estuary; equal sized reaches are specified up and downstream. Degradation, speciation, and adsorption processes are modeled in the same manner as the river and lake. Degradation rates are summed for the undissociated species of the contaminant. Suspended sediment concentrations must be input by the user.

Mills et al. (1982) describe a number of simplified techniques and models for estuarial simulation. Most are based upon the modified tidal prism to calculate the flushing time of a contaminant from the estuary. The Pritchard Box Model (Pritchard, 1969) is steady-state, and simulates the transport of conservative contaminants in a two dimensional (x,z) mode. It is designed for stratified estuaries and allows only continuous loading.

The TOX-SCREEN estuary model utilizes a simple solution to the advection/dispersion equation, similar to Pritchard's Box Model. It considers the estuary to be shallow and well mixed; thus salinity profiles and two-dimensional flow are not considered.

Important Advantages/Deficiencies. The estuary model is well-suited for shallow, well-mixed tidal rivers because of its uniform geometry and one-dimensional flow. Simulation of deep, stratified estuaries, or ones that are irregularly shaped or branching is not possible. The fresh water velocity is steady, which is not realistic over a long simulation period (>1 year).

4.1.4 Ocean Model

The ocean outfall model is based on a Gaussian type, linear diffusion model which estimates dispersion of pollutants discharged from a multi-port discharger. The model assumes steady, uni-directional flow, no re-entrainment of effluent back into the plume, movement of the resulting pollutant field at the same rate as the prevailing current, and negligible vertical and longitudinal mixing. The diffuser is represented as a line source perpendicular to the current flow. The equation to calculate the maximum, or plume centerline concentration (C_{max}) at any distance 'x' from the diffuser was taken from Brooks (1960).

The model is sensitive to the dilution factor used with the user-input effluent concentration to estimate the initial concentration (Co) after dilution. Pollutant concentrations of dissolved neutral, ionic, and adsorbed forms are computed in the same manner as the other water bodies, except that input mass to a specific water volume is not considered because compartments are not used.

The ocean outfall model is similar to one described in Mills et al. (1982). Both are designed for estuaries or coastal waters where the pollutant is discharged through submerged dischargers. The Mills et al. model utilizes dilution tables as a function of depth and Froude number created by a numerical plume model. Mills et al. also incorporate the degree of density stratification, port spacing, and depth into the dispersion coefficient, which the TOX-SCREEN model does not.

Important Advantages/Deficiencies. The reviewed ocean outfall model and the TOX-SCREEN ocean model utilize the same equations to determine effluent dispersion from a submerged diffuser. The primary deficiency of the TOX-SCREEN model may be the determination of the initial dilution factor. McDowell-Boyer and Hetrick (1982) give a conservative value of (0.02) for this factor based on empirical data, and do not correlate it to depth, which is the most critical and sensitive variable in the initial dilution term. No guidance is provided on how to adjust this factor according to depth.

4.2 PREVIOUS TESTING RESULTS

4.2.1 Comparison with Measured Data

Preliminary testing of the TOX-SCREEN aquatic model was performed by Oak Ridge Laboratory (Hetrick and McDowell-Boyer, informal report). The tests involved comparing simulated results for trichloroethylene (TCE) with observed concentrations near a production plant on the Mississippi River. The results are summarized below.

Comparisons were made for three scenarios: discharge into the river, discharge into an effluent canal from the plant, and at a settling pond weir. Due to lack of data, assumed values were used for loading rates and velocities in the second and third scenarios. Media interaction was considered by simulating concentrations in air due to volatilization and redeposition; however, measured air concentrations were not available. Table 4.1 lists the important input data common to the three scenarios, and Table 4.2 presents the input and results for specific scenarios.

Hetrick and McDowell-Boyer (informal report) concluded that the comparison was "fairly good" considering the input data uncertainties. Simulated concentrations were within a factor of two of measured values for two scenarios, and were overpredicted by a factor of fifteen for the other scenario. Apparently, the assumed loading and/or velocity (critical input parameters) for this scenario were not correct.

4.2.2 Comparison with EXAMS

Further testing of the TOX-SCREEN stream model was performed by Hetrick (1983c). In this test, TOX-SCREEN results were compared with EXAMS' (Burns et al., 1982) results for four different chemicals in the Delaware River. Also volatilization rate constants computed according to the recommended method in the TOX-SCREEN documentation (McDowell-Boyer and Hetrick, 1982) were compared with the pseudo first-order rates computed by the EXAMS model.

Input for the two models was essentially identical, and was based largely on the U.S. EPA Office of Toxic Substances, Graphical Exposure Modeling System (GEMS) (GSC, 1982) "user environment number 10" (Delaware River, Philadelphia). The dispersion pathways between EXAMS surface compartments, and advection from EXAMS bed sediment compartments to water column compartments were turned off since TOX-SCREEN does not model these processes. The chemicals modeled were methylene chloride, nitrobenzene, pentachlorophenol, and hexachlorobutadiene.

The predicted results of the two models for all chemicals were essentially identical; Hetrick (1983c) concluded that the small differences were due to the redeposition of volatilized chemical from air to water, which is simulated by TOX-SCREEN, and evaporative/rainfall water fluxes simulated by EXAMS. The close agreement between these models is expected, since they are essentially identical when EXAMS bottom compartments and dispersive processes are turned off, and when steady-state loading is assumed in TOX-SCREEN. Also, volatilization rate constants computed by the EXAMS model and by the recommended method in TOX-SCREEN (Southworth, 1979) were within a factor of two of each other.

TABLE 4.1 INPUT PARAMETERS FOR TCE TESTS (From Hetrick and McDowell-Boyer, informal report)

Parameter	Definition	Value
WKP, WKH	Photolysis, hydrolysis rate constants	6.2E-8 /s
WKV	Volatilization rate constant	5.56E-5 /s
SWKSW	Soil-water partition coefficient	15. l/kg
UDG	Dry deposition velocity	0.02 m/s
WRATG	Washout ratio	2.27
AK	Chemical degradation rate in air	1.6E-5 /s
UW	Wind speed	3. m/s

TABLE 4.2 INPUT PARAMETERS AND RESULTS OF TCE TESTING (From Hetrick and McDowell-Boyer, informal report)

	Scenario		
	1	2	3
Input			
WMINR (loading rate kg/s)	0.061	0.072	4.48E-4
WVELR (stream velocity m/s)	1.0	3.0	1.0
NR (number of reaches)	4	4	3
WLENR (reach length m)	250.	100.	100.
WWIDR (reach width m)	300.	30.	7.
WDEPR (reach depth m)	10.	5.5	1.5
Results (Conc. in last reach (ug/m^3))			
Simulated (Adsorbed)	0.83	167.	19.
Simulated (Dissolved)	1.9E4	1.4E5	4.2E4
Measured (Dissolved)	2.2E4	9.0E3	3.7E4

An additional comparison was made between the models with the EXAMS dispersive processes and bottom/surface compartment interactions simulated. In this test, predicted concentrations were within a factor of 1.3 of each other for both dissolved and adsorbed species. However, the comparison was shown only for methylene chloride which has a K_{OC} = 24. l/kg. Comparison of results for pentachlorophenol (K_{OC} = 26203. l/kg) or hexachloro- butadiene (K_{OC} = 3713. l/kg) would likely have indicated significant adsorption of chemical in bottom sediments.

4.3 CURRENT TESTING RESULTS

4.3.1 Introduction

The river, lake, and estuary models of TOX-SCREEN were tested by comparison against observed conditions and predictions of other models in four major scenarios. These scenarios are described in Table 4.3. The ocean outfall model was not tested but was evaluated and compared for consistency with other similar models. This information was provided in Section 4.1.5.

These test scenarios involved the use of just the aquatic models; simulations of inter-media processes between air-water and water-soil were not considered; hence, source terms were applied directly to the water body.

Descriptions of each test scenario follow, and include a description of the water body characteristics, parameter values used, model options considered, and evaluation of results compared to observed conditions and other model predictions.

4.3.2 Yazoo River Test

The Yazoo River test involved testing the river model of TOX-SCREEN against predictions from the models HSPF (Johanson et al., 1981), EXAMS (Burns et al. 1982), and WASP (Ditoro et al., 1982). These three models were compared as described in a study by Mulkey et al. (1982). In the study, flow and loading rates were alternated between steady state or time-varying, in different combinations for two chemicals. Chemical No. 1 exhibited high decay and low partitioning; Chemical No. 2 exhibited low decay and high partitioning.

TABLE 4.3 SCENARIOS TESTED WITH TOX-SCREEN AQUATIC MODELS

TOX-SCREEN Model	Waterbody	Compared with Other Models	References
River	Yazoo River, MS.	HSPF* EXAMS** WASP***	Mulkey et al. (1982)
River	Mississippi River, IA. RM 170	CPLUME	Schnoor et al. (1982)
Lake	Saylorville Reservoir, IA.	-	Leung et al. (1982)
Estuary	Newport Bay, CA.	WRE LINK NODE	Orlob 1981 Boutwell 1982

* Johanson et al., 1981
** Burns et al., 1982
*** Ditoro et al., 1982

TOX-SCREEN was executed for conditions of daily varying flow and steady loading. Application of TOX-SCREEN to these conditions was accomplished by obtaining steady-state solutions to the selected flow conditions in the same manner as was done for EXAMS. The variation in flows was small, as flow was regulated by an upstream reservoir. The general parameter values utilized for this test were derived from the EXAMS input, and suspended sediment concentrations were obtained from the simulated HSPF values. These data are shown in Table 4.4. In order to estimate the cumulative probability density function for chemical concentrations for these conditions the river velocity parameter was adjusted for each run according to the fraction of time the flow rate was less than or equal to the noted value. Flow values for the five EXAMS river segments were averaged for each frequency, and converted to velocities for input to TOX-SCREEN. River velocities and flows for the tests are provided in Table 4.5 along with the corresponding cumulative frequency for flow.

Fourteen runs were performed, seven for each chemical. Time series for each dissolved chemical as simulated by HSPF, WASP, EXAMS, and TOX-SCREEN are provided in Figures 4.1 and 4.2. The cumulative frequency in these figures represents the fraction of time the simulated chemical concentration was below the noted value; Mulkey et al., computed these distributions from time series of the dissolved chemicals as simulated by HSPF and WASP. Results for EXAMS and TOX-SCREEN are actually steady-state solutions to specific flow conditions, as described above. The river velocity frequencies were inverted (i.e., 1. - freq) for these two models to obtain the corresponding chemical concentration frequencies. It should be noted that the curves in Figures 4.1 and 4.2 for HSPF, WASP, and EXAMS were drawn using values from figures in the referenced study (Mulkey et al., 1982); consequently, the curves may not be entirely accurate.

Above the 70% level the TOX-SCREEN concentrations reflect the lower flows and higher residence times of the chemicals in the waterbody. Chemical 1 concentrations are lower than Chemical 2 from the 15% level up; indicating the greater effect of residence time on the more degradable pollutant. The curves for EXAMS and TOX-SCREEN are similar for both chemicals, as are the curves for HSPF and WASP.

The TOX-SCREEN results are very close to the other models as is expected; however, TOX-SCREEN generally overpredicts concentrations for both chemicals. In this case, the conservatism may be caused by the absence of sediment bed-water column interactions. A sediment bed would act as a

TABLE 4.4 PARAMETER VALUES FOR YAZOO RIVER TESTS

Number of reaches = 5

Reach length = 9.66 km

Reach width = 23.6 m (area/length for EXAMS segments)

Reach depth = 2.53 m (average of EXAMS Segment Depths)

Sediment concentration = 11.2 mg/l (average of monthly values computed by HSPF)

Chemical load = 7.64 kg/day

Chemical partition coefficient = 6.0 l/kg (Chemical 1)
60. l/kg (Chemical 2)

Chemical decay rate = 2.3E-6 /s (Chemical 1)
7.3E-7 /s (Chemical 2)

TABLE 4.5 RIVER VELOCITIES FOR YAZOO RIVER TESTS

% OF Time Flow < Value	Average Flow (m^3/s)	Velocity (m/s)
5	10.4	0.174
15	13.6	0.228
30	20.6	0.345
50	25.5	0.427
70	33.8	0.566
85	54.7	0.916
95	164.	2.75

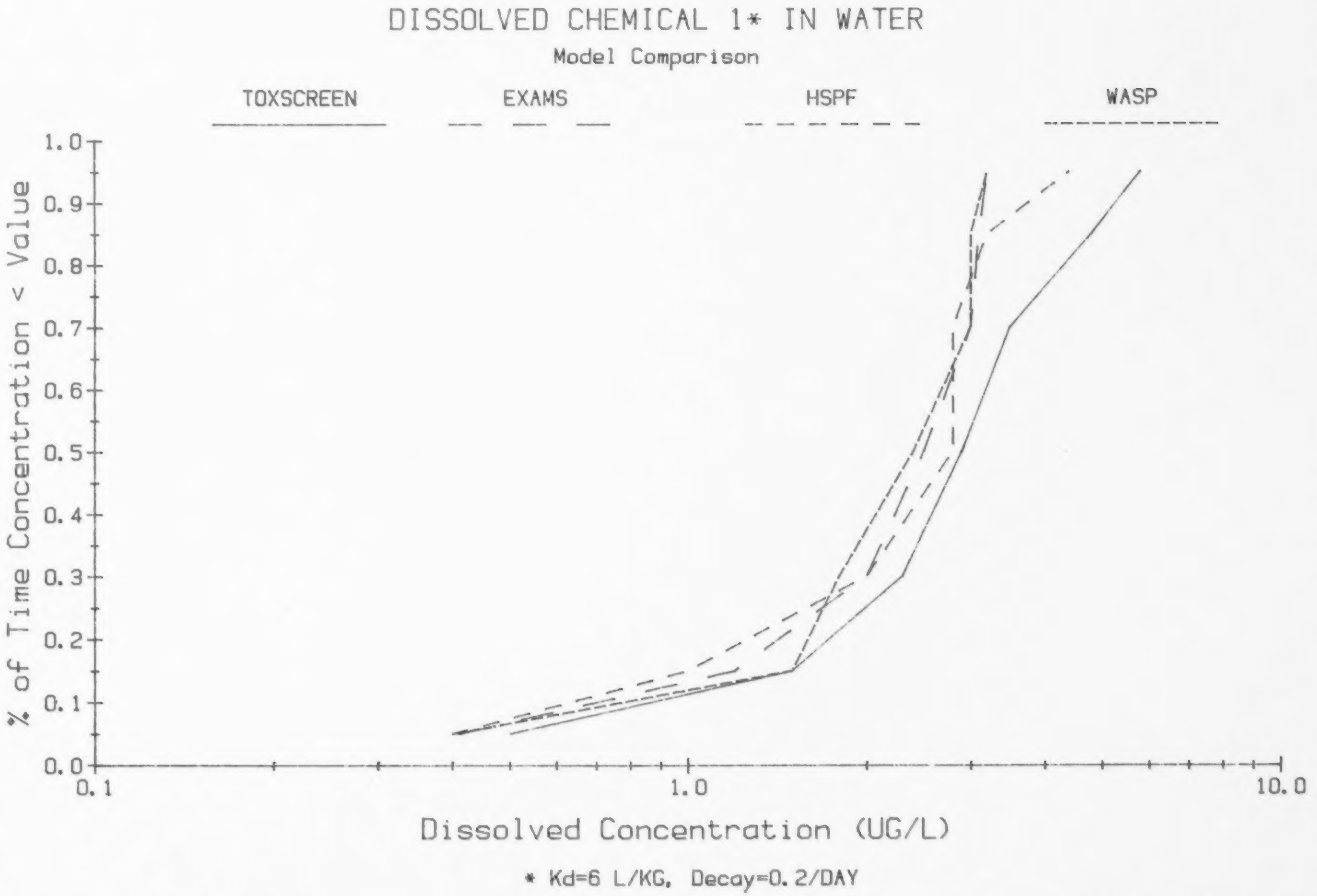

Figure 4.1 Comparison of TOX-SCREEN with EXAMS, HSPF, and WASP - Chemical 1.

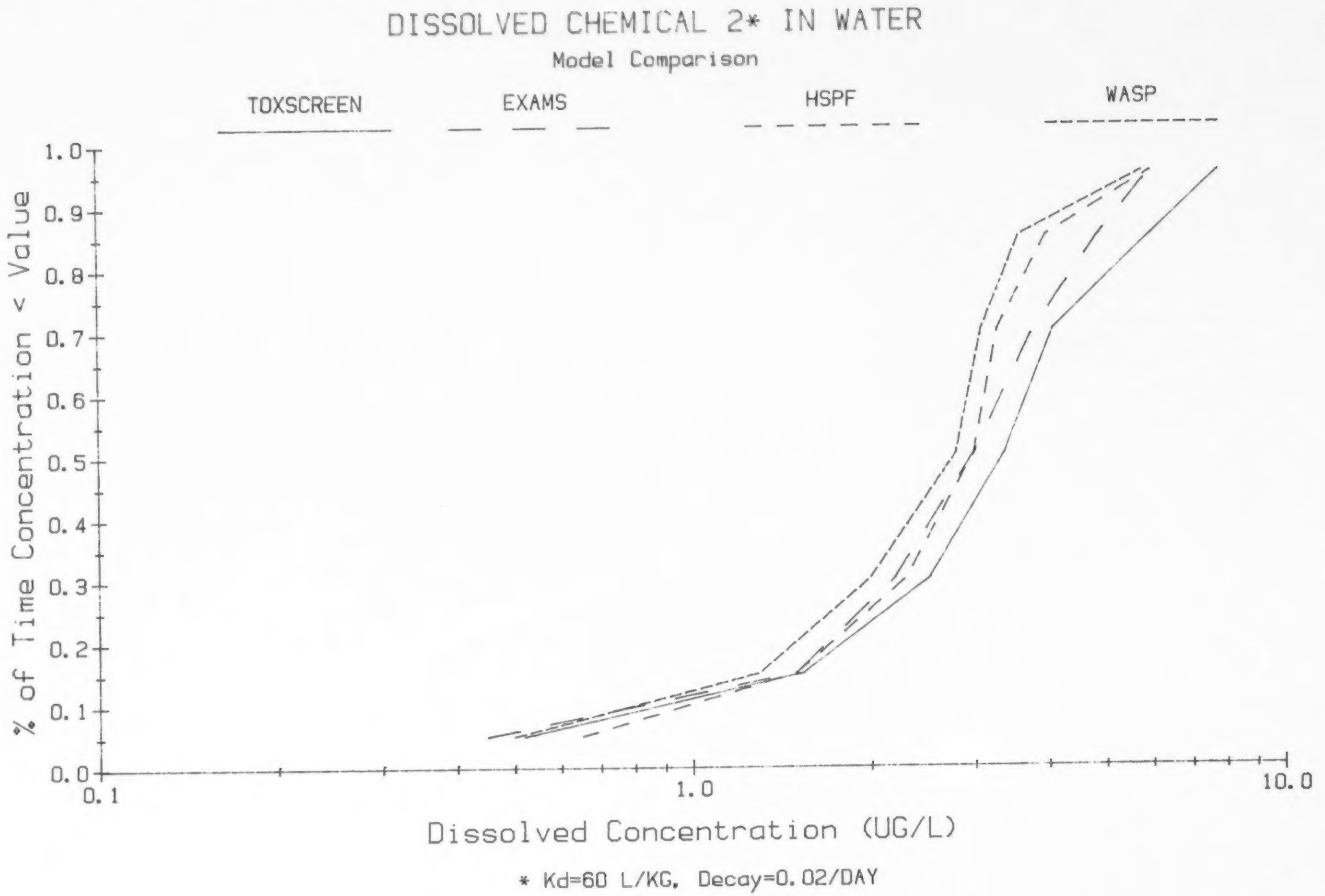

Figure 4.2 Comparison of TOX-SCREEN with EXAMS, HSPF, and WASP - Chemical 2.

sink for chemical, reducing the dissolved concentrations. Since EXAMS and TOX-SCREEN are very similar in their computational methods, the differences between these two models are due to the above effect and/or use in TOX-SCREEN of the average flow conditions for the five EXAMS segments. Overall, for the chemical characteristics and environmental scenario used in this test, TOX-SCREEN compared very well with the other models.

4.3.3 Mississippi River (RM170) Test

The TOX-SCREEN river model was also tested against observed data and results from the model CPLUME for ammonia-N at River Mile 170 on the Mississippi River. Model parameter values and observed data were obtained from Schnoor et al. (1982), who simulated the effects of suspended sediment and dissolved chemical dispersion from dredging operations. Parameter values used for TOX-SCREEN are presented in Table 4.6. These parameters were also used for CPLUME, a one-dimensional steady-state river model with a horizontal line source. A conservative simulation (after Schnoor) was performed (K_d = 0.0 and decay = 0.0). Two runs were made: 1) constant velocity and pollutant load, and 2) constant velocity and pulse (one month) loading. Comparisons were made between: 1) the first run, 2) the observed data, and 3) CPLUME results.

The results are presented in Figure 4.3. Because of the steady loading and flow conditions, and conservative chemical, TOX-SCREEN results did not vary spatially or temporally. They were however, slightly lower than the observed concentrations over most of the simulation period, and approximately two times larger than the CPLUME concentration at 250 m downstream.

Between CPLUME and TOX-SCREEN, the differences in concentration may be due to the fact that the calibration of CPLUME included increasing the dispersion coefficient, which caused a wider plume, but decreased chemical concentration rapidly downstream. This may also explain the difference between the observed conditions and CPLUME results. Overall, however, TOX-SCREEN shows good agreement with the observed conditions.

4.3.4 Saylorville Reservoir Test

The TOX-SCREEN lake model was tested with data from a

TABLE 4.6 PARAMETER VALUES FOR THE MISSISSIPPI RIVER (RM170) TEST (From Schnoor et al., 1982)

Number of reaches = 5

Reach length = 50 m

Reach width = 200 m

Reach depth = 4 m

River velocity = 0.8 m/s (steady)

Chemical load = 6.24E-3 kg/s (steady)

Chemical decay rate = 0.0 (conservative)

Chemical partition coefficient = 13.0 l/kg (sand)

Sediment density = 2.65 g/cm3

Sediment diameter = 0.4 mm

Slope = 1.3E-4 m/m

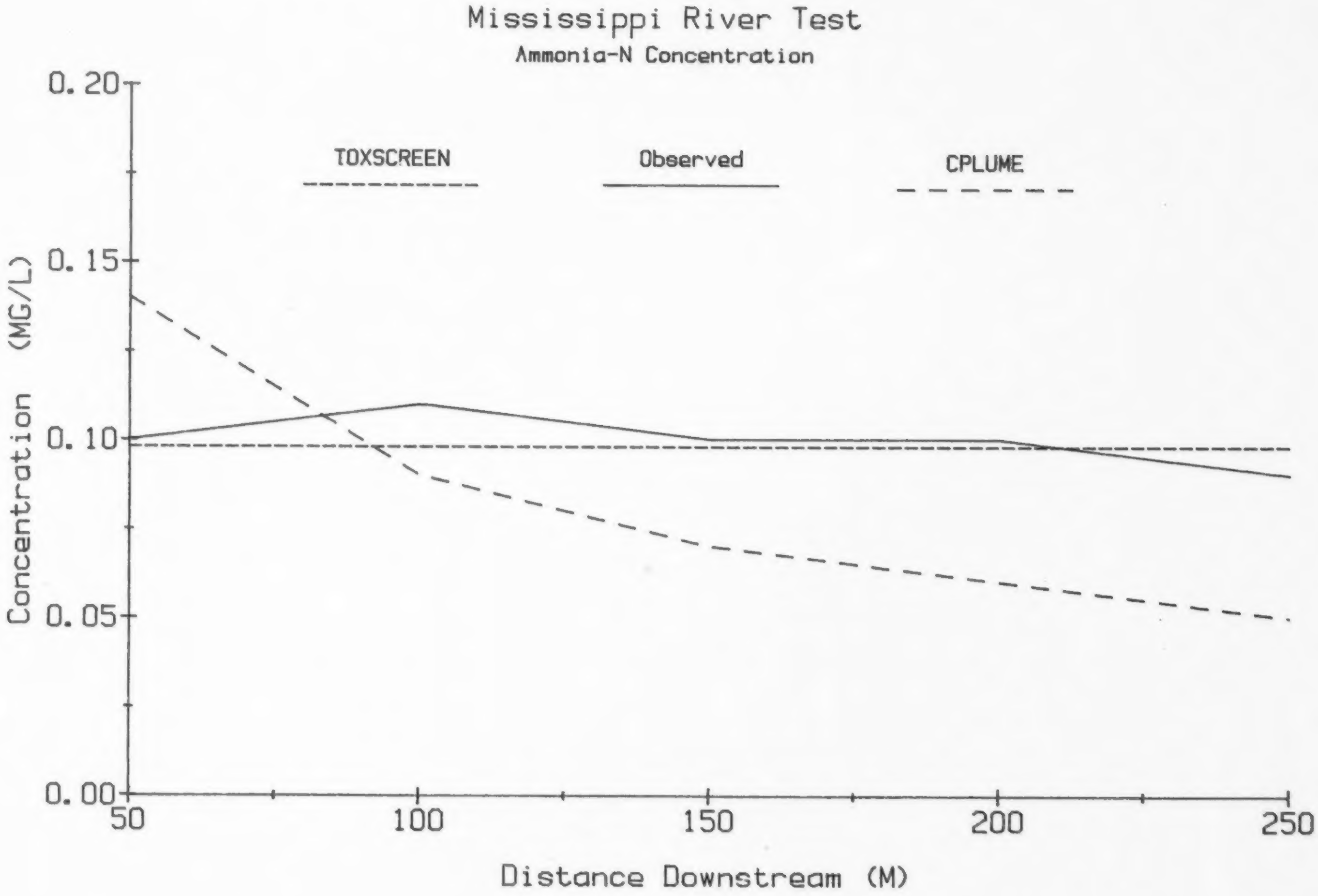

Figure 4.3 Ammonia-N concentrations in the Mississippi River - comparison of model results and observed data.

pesticide (dieldrin) accumulation study in the Saylorville Reservoir, a new impoundment on the Des Moines River (Leung et al., 1982). The purpose of that study was to determine the rate of pesticide deposition and the effects of impoundment on pesticide accumulation in different species of fish. Mean monthly concentrations of dieldrin were provided at two locations: upstream on the Des Moines River, and in the reservoir, for both the dissolved and the adsorbed fractions.

Hydrologic data, including monthly flow velocities, were obtained from a USGS discharge summary for a station immediately upriver from the reservoir. The monthly flow velocities were averaged for the year, yielding a value of 0.5 m/s. This was done to facilitate simulation of suspended sediment concentrations and trapping efficiency of the reservoir. Some of the monthly flow velocities would not have been high enough to overcome the Shields factor in Laursens formula (1958), which represents the limit below which particles will not move. Table 4.7 is a list of parameter values for the Saylorville Reservoir test. Table 4.8 contains the monthly loading rates of dieldrin into the Saylorville Reservoir. Figure 4.4 presents the observed and simulated monthly concentrations of dissolved dieldrin in the reservoir; Figure 4.5 shows the results for the total concentration of dieldrin (dissolved + suspended).

In Figure 4.4, TOX-SCREEN results for the dissolved fraction correspond fairly well with the observed data over the simulation period, showing a maximum ratio of 3.1. Given the uncertainty in the observed values, which were reported to one significant digit, and use of a constant average velocity for all months of the simulation, the results appear surprisingly good.

In Figure 4.5, TOX-SCREEN consistently underpredicts the total dieldrin concentrations over the simulation period, particularly in the first month, where they differ by a factor of 3.8. This difference could be caused by a number of factors including those mentioned above. Another possible source is the confusion over the input lake velocities described in Section 4.1.2. Use of the upstream river velocities overestimates the lake velocity and underestimates the hydraulic detention time causing low predicted concentrations.

While the above comparison is still within the bounds of a "screening" model, inspection of the relative amounts of dissolved and adsorbed dieldrin showed that the adsorbed fraction was dramatically underpredicted. Because of the constant velocity used in the simulation, and the resulting

TABLE 4.7 PARAMETER VALUES FOR SAYLORVILLE RESERVOIR TEST

Surface area of lake = 2.2E+4 m2

Depth of lake = 4.3 m

Chemical decay rate = 0.0 /s

Dieldrin partition coefficient = 11000. l/kg

Lake water velocity = 0.5 m/s (average of monthly values for USGS gage on Des Moines River above reservoir)

Median sediment diameter in tributary = .45 mm

Sediment density in tributary = 2.65 g/cm3

Depth of tributary = 2.0 m (from USGS data)

Slope of tributary = .00013 (From USGS data)

TABLE 4.8 MONTHLY LOADING RATES OF DIELDRIN INTO SAYLORVILLE RESERVOIR

Month (1977-1978)	Loading Rate (kg/s)
October	7.4E-7
November	3.7E-7
December	2.1E-7
January	1.1E-7
February	1.5E-7
March	5.1E-7
April	9.3E-7
May	5.3E-7
June	1.4E-6
July	1.3E-6
August	4.1E-7
September	8.7E-7

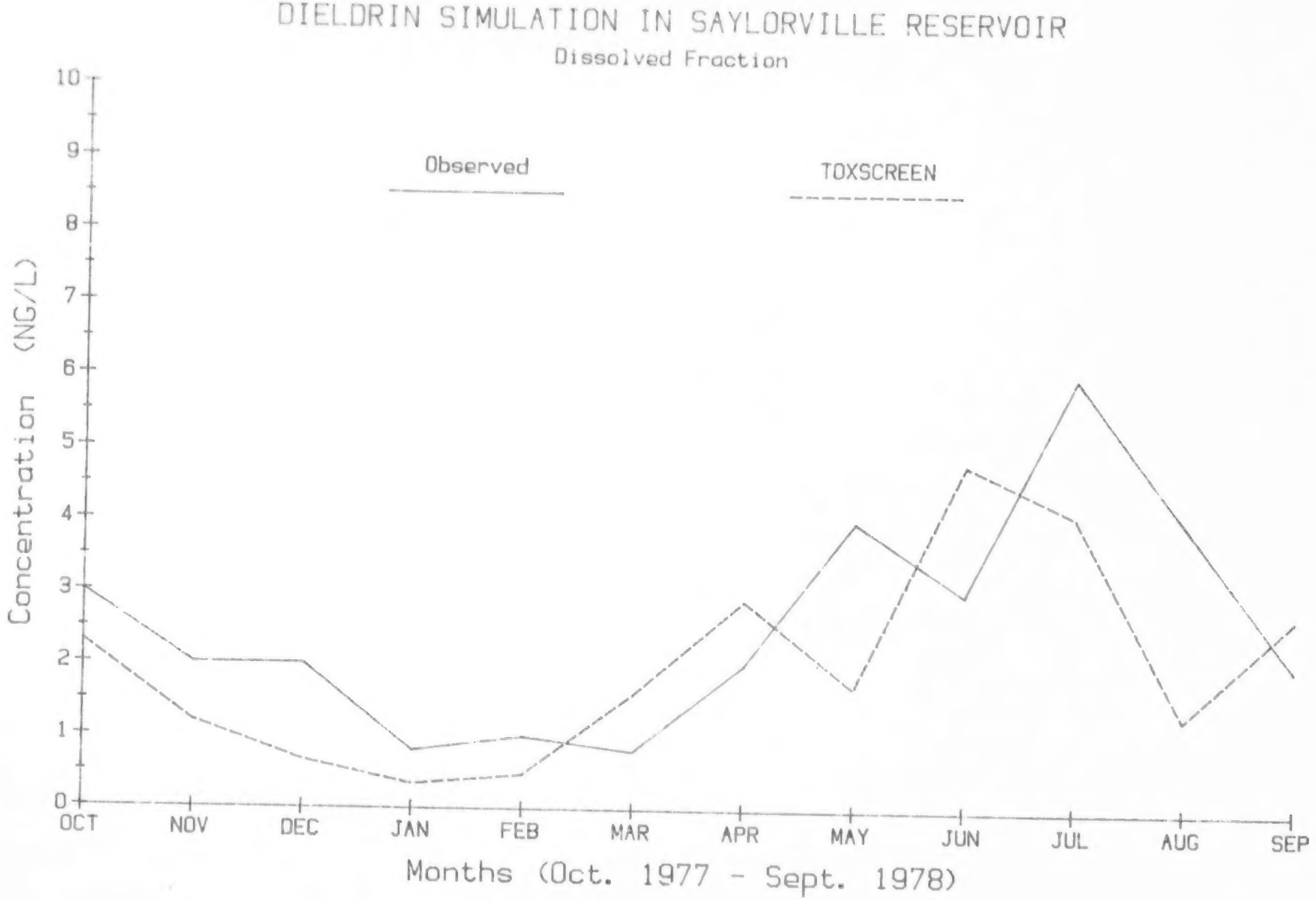

Figure 4.4 Dissolved Dieldrin in Saylorville Reservoir - comparison of TOX-SCREEN to observed data.

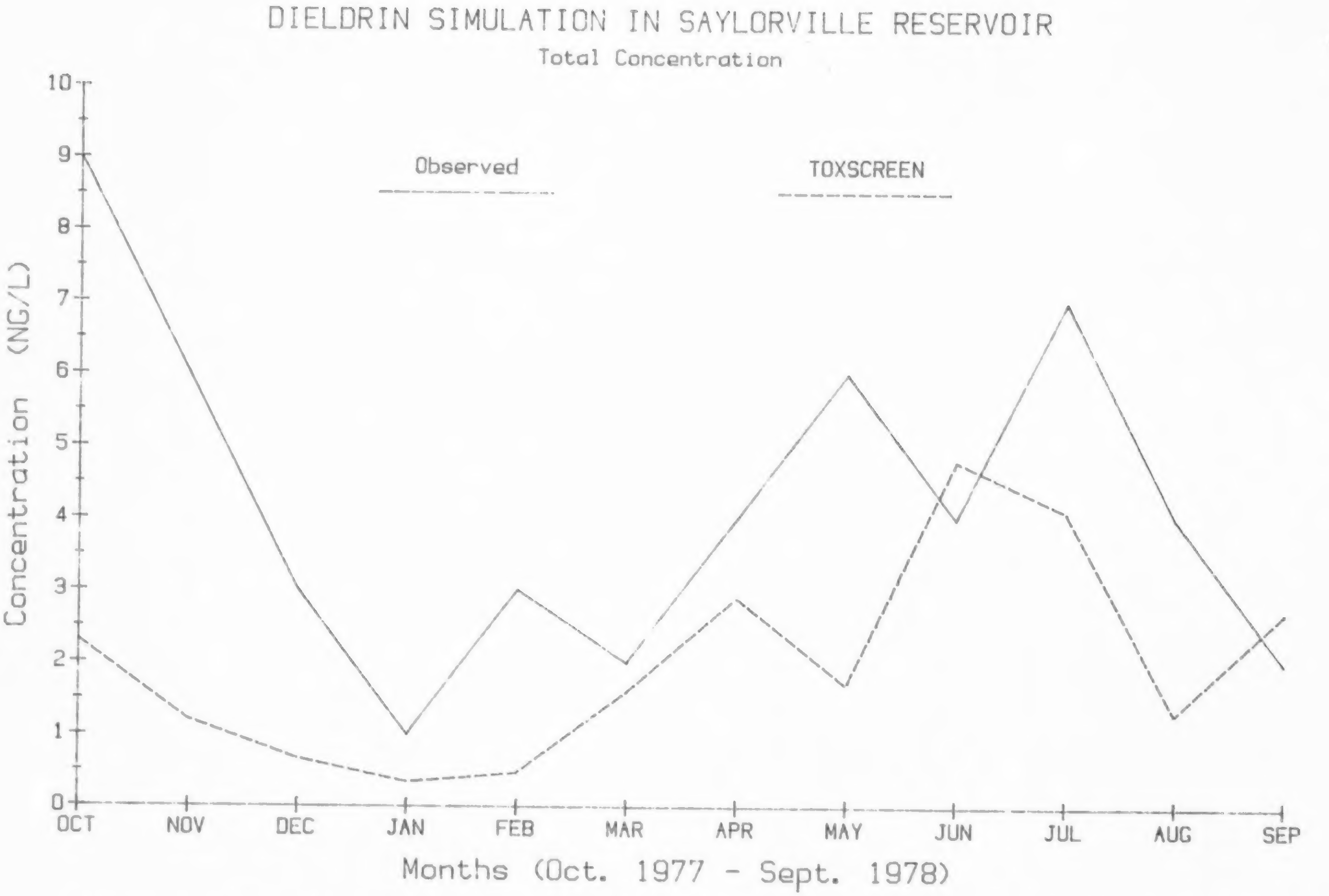

Figure 4.5 Total Dieldrin in Saylorville Reservoir - comparison of TOX-SCREEN to observed data.

constant suspended sediment concentrations, the simulated ratio of dissolved to adsorbed dieldrin remained constant at a value of 236, whereas the observed value for this ratio varied from 6.0 to 0.5. A possible cause for this discrepancy is a low value of the sediment-water partition coefficient for dieldrin; however the value used (1.1E4) should be appropriate. Apparently, the simulated suspended sediment concentrations were much too low resulting in low adsorbed fractions. Either the input flow velocity was too low (Laursen's formula is not accurate for such flow conditions), or the trapping efficiency, which is taken from a curve based on lake inflow and volume in subroutine SEDLOW, is too high for this reservoir.

4.3.5 Newport Bay Estuary Test

The TOX-SCREEN estuary model was tested by comparison against results from a steady-state link-node model simulation of a non-conservative pollutant in Newport Bay, CA. Hydrodynamic parameters were obtained from a case study using the link-node models (Orlob, 1981), and source parameters and observed data were obtained from Boutwell (1982).

The branching Newport Bay Estuary was simplified to TOX-SCREEN's specifications by assuming: no branching, utilize main channels from headwaters to the mouth; average width of utilized channels; and total length of the estuary was based on the sum of channel lengths from the headwaters to the mouth. Table 4.9 is a list of the parameter values selected for the test.

Figure 4.6 presents the concentration profile over the length of the estuary for both the link-node and TOX-SCREEN models. The chemical loading was steady and was input at point '0'. A high degradation rate was applied (.63/day), and the adsorption coefficient was zero. TOX-SCREEN results are in good agreement with the results from the steady-state link-node model upstream of the point source. Downstream of the source at the mouth, TOX-SCREEN results are approximately three times as high as those of the link-node model, but are still within range of acceptability for screening level assessments.

TABLE 4.9 PARAMETER VALUES FOR NEWPORT BAY ESTUARY TESTS
(From Orlob, 1981)

Length of estuary (from headwaters to mouth) = 10.64 km

Average width = 275. m

Average depth = 2.35 m

Maximum tidal velocity = 0.49 m/s

Longitudinal dispersion coefficient = 150 m^2/s

Chemical loading rate = 8.47E-4 kg/s (From Boutwell, 1982)

Chemical decay rate = 7.3E-6 (From Boutwell, 1982)

Chemical partition coefficient = 0.0 (From Boutwell, 1982)

Number of reaches = 20

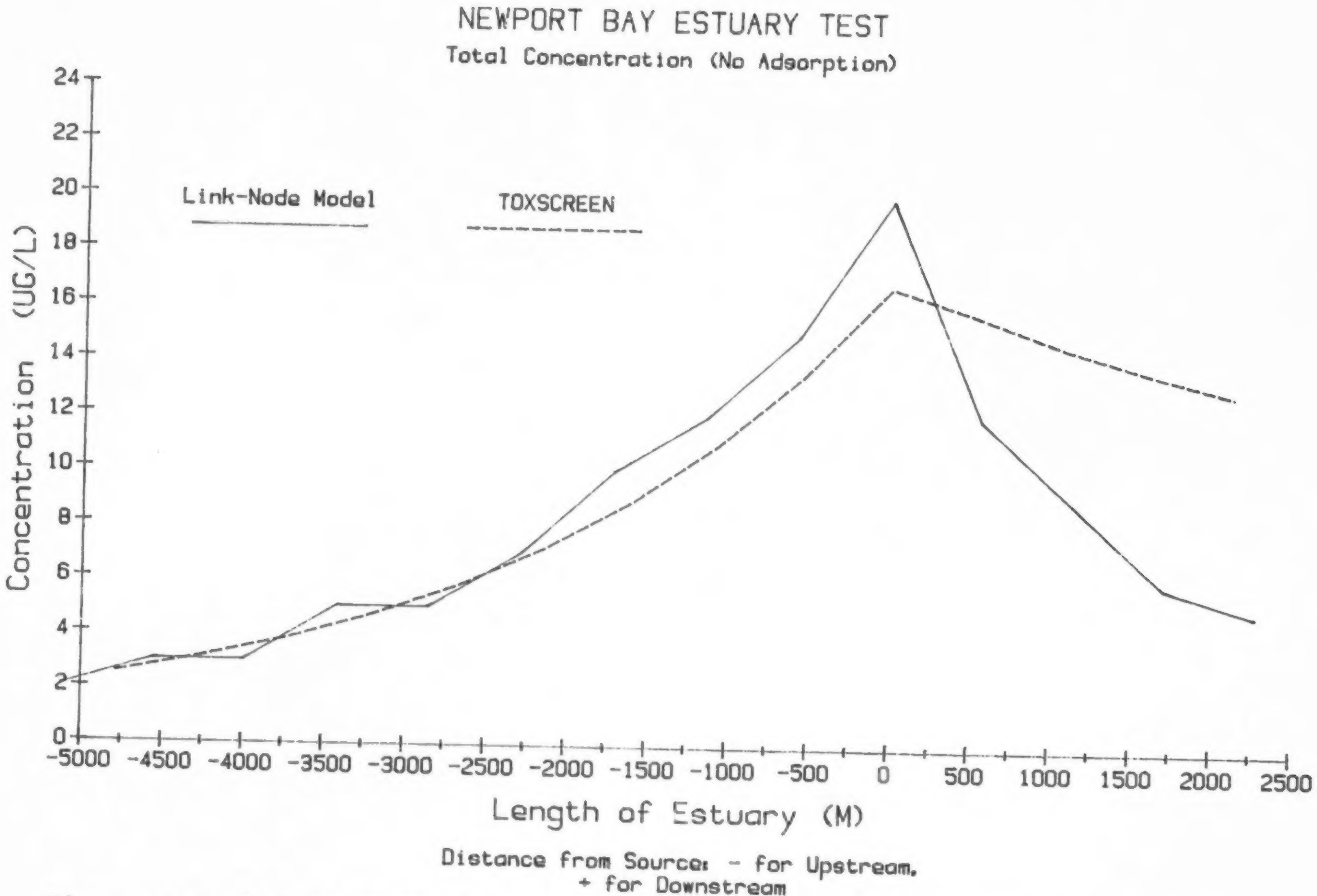

Figure 4.6 Non-conservative pollutant in Newport Bay Estuary - comparison of TOX-SCREEN to Link-Node model.

4.4 CONCLUSIONS

Based on critical review of the models, and analysis of both previous and current testing efforts, a number of conclusions are apparent regarding the TOX-SCREEN aquatic models. Generally, the model tests accurately predicted dissolved pollutant fractions and those with low sediment-water partition coefficients. The tests and review suggest that the models are appropriate for screening of chemicals that do not absorb to a large extent; TOX-SCREEN users should be wary of predicted results for chemicals with high K_d's. While adsorption/desorption and other interactions with bed sediments were not important in most of the tests described here, these effects will be much more critical for high K_d chemicals and in long-term simulations of reservoir/lake water quality. Also, inaccurate suspended sediment concentrations predicted for low flowing rivers and lakes may have a detrimental effect for simulation of highly adsorbed chemicals.

The estuary and ocean models also appear to be appropriate for use in TOX-SCREEN, although generally estuary geometry has to be simplified so that the system resembles a tidal river because of the uniform segment requirements. Estuary testing results were good; TOX-SCREEN predicted higher concentrations near the mouth than did the compared model. This may be due to the steady fresh water velocity which is used in the advection/dispersion equation for each point away from the source. This may cause higher concentrations downstream over the course of a tidal cycle.

While no test of the ocean model was performed, the sensitivity to the user-specified dilution factor is an apparent drawback that could be corrected by a slight modification of the method (Mills et al., 1982). However, limited anticipated use of TOX-SCREEN for assessments near ocean outfalls suggests that these changes are relatively unimportant.

A summary of specific conclusions and recommendations for various water body models includes:

Rivers and Lakes:

- Incorporation of simple sediment bed compartments with the processes of diffusion, adsorption/desorption, erosion/deposition, and burial, while operationally difficult, would make the river and lake models more complete. Ditoro et al. may provide an example.

- The suspended sediment computational method does not operate at low stream velocities. More guidance to the model user regarding this subject, and extension of the methods to low velocities would be useful. Printing of suspended sediment concentrations in the output would also be helpful.

- Use of input flow velocities to compute hydraulics is less appropriate than flow rates, and also causes the confusion regarding lake hydraulics (Section 4.1.2). If the model developers determine that actual velocities are needed (for suspended sediment concentration calculation), then TOX-SCREEN could require flows and velocities.

Oceans:

- Provide more user-guidance for determination of initial dilution factor.

SECTION 5

INTERMEDIA TRANSFER

Simulation of intermedia transfer between air, water, and soil requires that processes which drive the transfer across media interfaces be simulated as well as defining the locations of water bodies and soil surfaces relative to atmospheric pollutant sources. This section is an evaluation of the methods used in TOX-SCREEN to effect intermedia transfer. Figure 1.1 in Section 1.2 depicts the intermedia and intramedia processes simulated in TOX-SCREEN.

5.1 REVIEW AND EVALUATION

Intermedia transfer in TOX-SCREEN is dominated by the following concepts:

1) Most of the basic physical/chemical processes which drive chemicals across media boundaries are considered in TOX-SCREEN, and are represented by simplified deterministic models or empirical equations. These processes are wet and dry atmospheric deposition, volatilization, surface and ground-water runoff, and soil erosion by water and wind.

2) TOX-SCREEN is a true multimedia model because it considers two-way chemical transfer between media rather than the one-way transfer allowed in other recently developed multimedia programs such as UTM-TOX (Patterson et al., undated), HSPF (Johanson et al., 1981), and ALWAS (Tucker et al., 1981).

3) TOX-SCREEN is also unique in its use of generic environments to define the relative sizes and locations of pollutant sources, environmental media, and media interfaces.

5.1.1 Processes

Atmospheric Deposition. Deposition of pollutant from the air to water and soil surfaces considers dry and wet deposition processes separately. It also allows the user to distinguish between particulate and gaseous pollutants. If the chemical is specified as a particulate, TOX-SCREEN assumes that pollutant which volatilizes from the soil or water is in the gaseous state. The rate of dry deposition of pollutant onto water or soil is given by:

$$D_{dry} = X_{ave} \cdot Vd \tag{5.1}$$

where D_{dry} = deposition rate of particulate or gaseous pollutant ($ug/m^2/s$)
X_{ave} = average ground-level air concentration of particulate or gaseous pollutant (ug/m^3)
V_d = dry deposition velocity of particulate or gaseous pollutant (m/s)

For wet deposition, washout ratios are used to estimate the flux as follows:

$$D_{wet} = X_{ave} \cdot P \cdot Wr \tag{5.2}$$

where D_{wet} = deposition rate of particulate or gaseous pollutant ($ug/m^2/s$)
P = precipitation rate (m/s)
Wr = washout ratio of particulate or gaseous pollutant ((ug/m^3) rain/(ug/m^3) air)

(It should be noted that Equations 5-1, 5-4, and 5-6 in McDowell-Boyer and Hetrick (1982) imply that the total deposition is computed (incorrectly) from the respective sums of the particulate and gaseous deposition velocities and washout ratios. For example, Eqn. 5-4 in that document states that the total wet deposition is given by:

$$D_{wet} = X_{ave} * P * (Wr,p + Wr,g) \tag{5.3}$$

However, inspection of the code indicated that gases and particulates are treated separately.

The above equations are simplified representations of the standard deposition-velocity and washout-ratio formulations of pollutant deposition to surfaces. The major uncertainties with their use are found in the evaluation of the input parameters. Deposition velocities depend strongly on wind speed, atmospheric stability, surface roughness, and particle characteristics (Eisenreich et al., 1981), and range from 0.01 to 10 cm/s for gases and 1.E-2 to 10 cm/s for particulates (Slinn et al., 1978). Washout ratios vary with particle size, drop size, and Henry's constant for the chemical, and range from 1.E5 to 1.E6 for particulates and 1 to 1.E4 for organic gases (Scott, 1981).

As a guide to the model user, single typical values of each of the velocities and washout ratios are provided in Appendix C of MBH. Since the deposition parameters are important to a reasonable prediction of the environmental distribution of atmospheric pollutants, a table of known values for specific chemicals or typical values for classes of chemicals would be very useful.

Volatilization. Pollutants may volatilize into the air from both water and soil. For water, a user-supplied volatilization rate constant is used with the mass of dissolved, neutral form of the chemical in the water to compute the flux. Again, this formulation is a simple and reasonable description of volatilization, provided that the input rate constant is reasonable. These rates depend strongly on water depth and turbulence and the chemical's Henry's law constant. Appendix C in MBH provides an appropriate estimation method (Southworth, 1979), which accounts for these factors.

Volatilization from soil uses a more detailed model by Farmer et al. (1980) which accounts for diffusion of pollutant from a contaminated layer through a cover layer of clean soil (Bonazountas and Wagner, 1981). The model is appropriate to describe pollutant losses where diffusion is the rate controlling process rather than volatilization from soil water or evaporation of pure chemical from the surface. The equation used in TOX-SCREEN (SESOIL) is:

$$Vs = Da \cdot [(n-\theta)^{10/3}/n^2] \cdot [C \cdot H/(R \cdot T \cdot L)] \qquad (5.4)$$

where
Vs = total volatilization flux (ug/cm^2/s)
Da = diffusion coefficient of chemical in air (cm^2/s)
n = total soil porosity (-)
θ = soil moisture (-)
C = chemical concentration in soil moisture (ug/ml)
H = Henry's Law constant (m^3 atm/mole)

R = gas constant (8.2E-5 m^3 atm/mole/K)
T = temperature (K)
L = cover soil thickness (cm)

There are three apparent limitations of this model. First, it assumes that the chemical is buried below a clean soil layer. The depth of this layer is assumed to be the depth to the middle of the particular SESOIL layer being considered. Thus the depth of burial will be unrealistic for pollutants applied to the surface such as from spills or atmospheric deposition, or when a narrow band of contaminated soil is located near the top or bottom of a thick SESOIL layer. The former effect can be reduced by using a thin top soil layer.

The second limitation is the mathematical dispersion inherent in SESOIL pollutant computations as a result of using only three layers in the soil column (see Sections 3.3, 3.4) This dispersion generally results in low predictions of the chemical concentrations in any layer. Both of these limitations will cause the volatilized mass of pollutant to be underpredicted for surface applied pollutants.

The third limitation, discussed by Wagner et al. (1983), is that the volatilization is allowed to occur from any layer. They suggest cut-off of volatilization at some arbitrary depth such as 2 m. However, as is discussed in Section 3, the layering scheme of SESOIL may also cause unrealistic volatilization.

The Farmer et al. (1980) model is a generally accepted soil volatilization model for buried chemicals. It is limited here by the surface application scenario and the limitations imposed by the SESOIL layering scheme. These limitations can be reduced by increasing the number of soil layers in SESOIL, and by providing appropriate guidance on selection of soil layer depths. Also, a simple and more appropriate model could be considered for estimating volatilization losses from surface-applied chemicals, such as the method proposed by Swann et al. (1982).

Soil Erosion. Since the stand-alone version of SESOIL does not simulate the processes of sediment erosion by water and sediment resuspension by wind, these values are estimated by empirical equations. For soil erosion, the following relationship is used (Langbein and Schumm, 1958):

$$G = (7.0 * P^{**}2.3) / (1 + 0.0007 * P^{**}3.3) \qquad (5.5)$$

where G = soil yield ($g/m^2/yr$)
P = annual precipitation (in)

The soil yield is coupled with the adsorbed pollutant concentration in the upper soil zone to obtain the eroded pollutant mass. This value is subject to much uncertainty because of variations in soil, topography, and vegetation.

For wind resuspension, empirical dust loading values provide estimates of the amount of surface soil contained in the air above the land due to wind erosion. Combining these values with the adsorbed pollutant concentration, the pollutant loading to the air is estimated by:

$$Xr = 10^{**}-6 * R * Su \tag{5.6}$$

where Xr = pollutant concentration in air due to wind erosion (ug/m^3)
R = empirical dust loading factor ($ug\ soil/m^3\ air$)
Su = adsorbed pollutant concentration in upper soil zone (ug/g)

Again, the application of empirical values leads to much uncertainty. An average R value of 38 ug/m^3 for non-urban areas and values from 33 to 254 ug/m^3 for urban areas reflect this variability (McDowell-Boyer and Hetrick, 1982), which is caused partly by the large quantities of industrial particulates in urban air. A value of 100 ug/m^3 is recommended as a default in TOX-SCREEN (Healy 1980).

It should be noted that the wind resuspension model does not provide a chemical flux term since only the concentration of soil (R), and thus chemical (Xr) in air is given by the empirical equation.

Runoff. Soil contributes pollutant to surface water via advection by surface and ground-water runoff in addition to the erosion discussed above. The respective fluxes from each soil zone are given by the product of the runoff volume and dissolved pollutant concentration, both of which are computed by SESOIL.

Estimation of runoff volumes in SESOIL is intrinsic to the fundamental hydrologic theory of that model, and cannot be adequately discussed here. The reader is referred to the SESOIL User's Manual (Bonazountas and Wagner, 1981). However, that theory is developmental, and has not been adequately validated. It has been reviewed and tested (Watson and Brown, 1984).

While the pollutant concentrations in soil-water also depend on the SESOIL hydrologic cycle, review and preliminary testing of the pollutant cycle in SESOIL have led to several conclusions questioning the appropriateness of model predictions of transport to ground water. These conclusions are discussed in Section 3.3.

5.1.2 Generic Environments

TOX-SCREEN utilizes a number of generic environmental scenarios to specify the sizes and relative locations of media as well as the locations of atmospheric pollutant sources. These scenarios depend on user-specified options such as type of water body (river, lake, estuary, or ocean coastal zone) and type of atmospheric pollutant source (point or area). The following discussion is based largely on the TOX-SCREEN documentation (McDowell-Boyer and Hetrick, 1982; and Hetrick and McDowell-Boyer, 1984).

If an atmospheric point source is simulated, the possible media interaction scenarios are defined as shown in Figures 5.1 and 5.2. The water and/or soil contaminated by the point source plume is delineated by the shape and size of the plume which intercepts the soil and water surfaces. The width of the plume is given by $4\sigma_y$ (σ_y = horizontal dispersion coefficient) which is computed by the atmospheric model. The locations of Xmax and Xfinal are specified as follows: Xmax, which is the distance from the source to the point of maximum ground-level concentration (computed by atmospheric model), is assumed to be the upstream end of the river/estuary/soil or the near edge of the lake; Xfinal is the downstream end of the river/estuary or the furthest extent of the lake's watershed. The wind direction is assumed constant, so that the plume is permanently oriented along the river/estuary or over the lake, resulting in the worst-case (conservative) scenario.

If an area source is simulated, the total area impacted by the source is user-specified, and the water bodies and/or soil areas are contained within the area. Figure 5.3 depicts the area source environment in TOX-SCREEN. Since the deposition due to an area source is assumed uniform over the area, locations of soil and water surfaces within the area are unimportant (McDowell-Boyer and Hetrick, 1982).

Volatilization from soil and water are summed and assumed to contaminate the air directly above their total areas only.

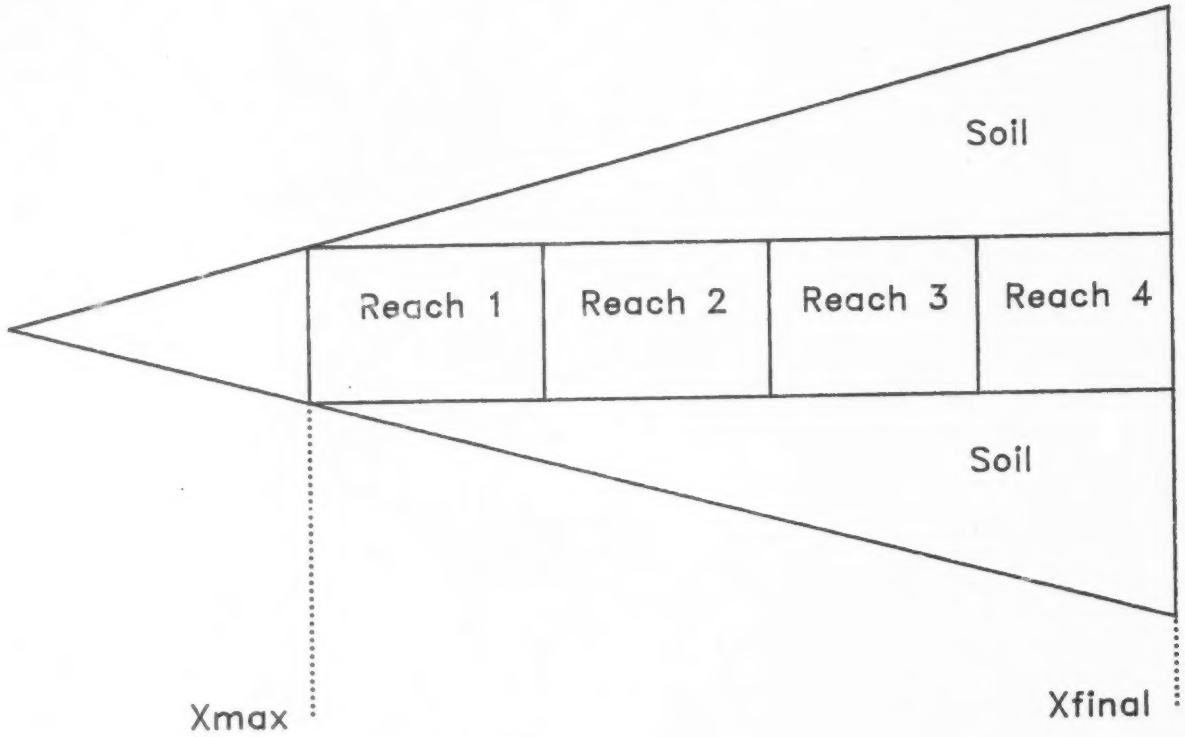

Figure 5.1 Generic Environment for Atmospheric Point Source, River, and Soil.(McDowell-Boyer and Hetrick, 1982)

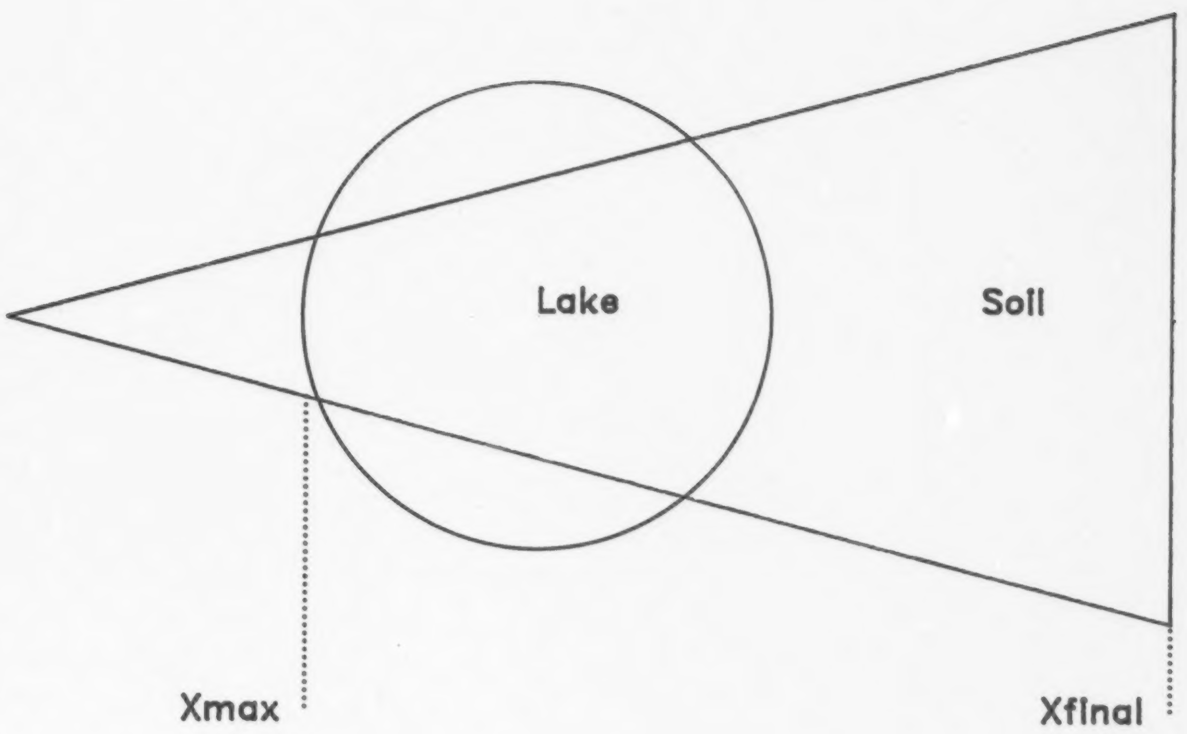

Figure 5.2 Generic Environment for Atmospheric Point Source, Lake and Soil. (McDowell-Boyer and Hetrick, 1982)

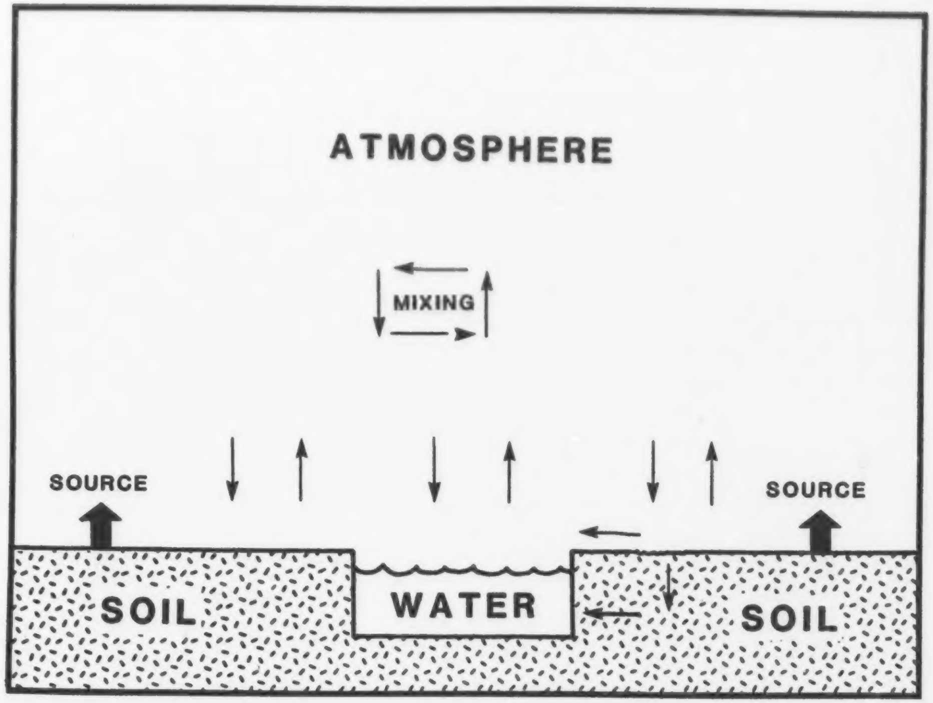

Figure 5.3 Atmospheric Area Source Generic Environment in TOX-SCREEN Showing Pollutant Movement

This area is thus treated as a separate area source, and the total pollutant concentration in the air directly above it is the sum of the concentrations due to the user-specified pollutant air source and the volatilization area source.

Soil areas are always assumed to be adjacent to surface water bodies. This results in computed surface runoff and erosion pollutant losses from land, and pollutant transported to ground water (computed in the SESOIL model) being immediately added to the water body, i.e., ground-water pollutant fate and transport are not modeled.

The media interaction processes and other factors which either increase the net pollutant flux between two media or increase the rate of transfer, do not necessarily result in conservative predictions since gain of pollutant by one medium is due to loss from the other medium. However, the use of generic environments, such as constant wind direction and plume locations over water bodies and soil areas, are conservative, since they result in higher simulated concentrations in one or more media without corresponding decreases in other media. The use of these environments in TOX-SCREEN is also appropriate to a screening model since they significantly reduce the required input.

5.2 SENSITIVITY TESTING

Since atmospheric deposition is the only mechanism for transfer of atmospheric pollutants to ground, sensitivity tests of the deposition parameters were performed to determine how they varied over ranges of typical values, and whether the default values produced any obvious biases or incorrect trends in the deposition. The dry deposition velocity and washout ratio parameters were independently varied over their respective ranges, while other parameters were held constant. For each parameter tested, the other deposition parameter was kept constant at zero or at its default value. Typical ranges of parameters were obtained from McMahon and Denison (1979), Eisenreich et al. (1981), Scott (1982), and Slinn et al. (1982). Default values were obtained from McDowell-Boyer and Hetrick (1982). The predicted surface deposition fluxes (wet, dry, and total), in units of mg/m^2, were plotted to observe the trends.

The scenario used for these tests was based on the TOX-SCREEN application (Southeast Ohio Study Area) described in Section 6, and consisted of a pollutant point source with the resulting plume oriented over river and soil surfaces. The source loading rate and meteorological input (wind speed, precipitation, etc) were taken directly from the Southeast Ohio application. Volatilization and other surface-to-air transfer processes were turned off so as to simplify the scenario and look only at the one-way deposition fluxes. The values of the test variables for all runs are shown in Table 5.1.

Figures 5.4 - 5.7 show the results of the tests. Figures 5.4 and 5.6 represent simple situations where only dry or wet deposition is operable, and the deposition rate first increases with velocity, and then decreases as the plume is depleted. This depletion is presumably due to deposition in the region upwind of Xmax where the plume has not yet mixed to the ground. While this effect may be correct, this deposition would in "reality" impact part of the geographic area under consideration by the model user, i.e. close to the source. For both wet and dry deposition the rate is very sensitive to the deposition parameter in the range from 0 to the TOX-SCREEN default/recommended value. Also, the TOX-SCREEN defaults are found to correspond fairly well to the maxima of the curves, thus maximizing predicted deposition.

Figures 5.5 and 5.7 represent situations where wet and dry deposition are competing. In these tests one of the parameters was held constant at its default value while the other was varied. The curves generally indicate the same behavior as in the single process case, with the added effect of the competition. For example, in Figure 5.5, dry deposition increases and wet deposition decreases as the dry deposition velocity increases up to approximately 1 cm/s. Then presumably, the loss mechanisms upwind of Xmax dominate and both rates decrease due to decreasing simulated average concentrations.

5.3 CONCLUSIONS

The basic process models which are used in TOX-SCREEN to compute intermedia transfers are generally physically sound and appropriate to a screening model. The critical deposition parameters are somewhat sensitive at values slightly below their recommended values. The empirical equations used to represent wind and water soil erosion are somewhat weak, but would primarily impact high-Kd chemicals. Also, implementation of the process models in TOX-SCREEN often results in decreasing their accuracy; for example, the layering scheme in SESOIL apparently impacts the volatilization model, and should be modified (See Section 3).

TABLE 5.1 VALUES OF THE TEST PARAMETERS FOR SENSITIVITY TESTS OF ATMOSPHERIC DEPOSITION

Figures 5.4 and 5.5

Dry deposition velocity (m/s)	0.0	.0005	.001	.005	.01	.025	.05	.075	.10
Washout ratio	0.0	5.E+5							

Figures 5.6 and 5.7

Washout ratio (*1.E4)	1.	10.	25.	50.	75.	100.	500.	1000.
Dry deposition velocity	0.	0.01						

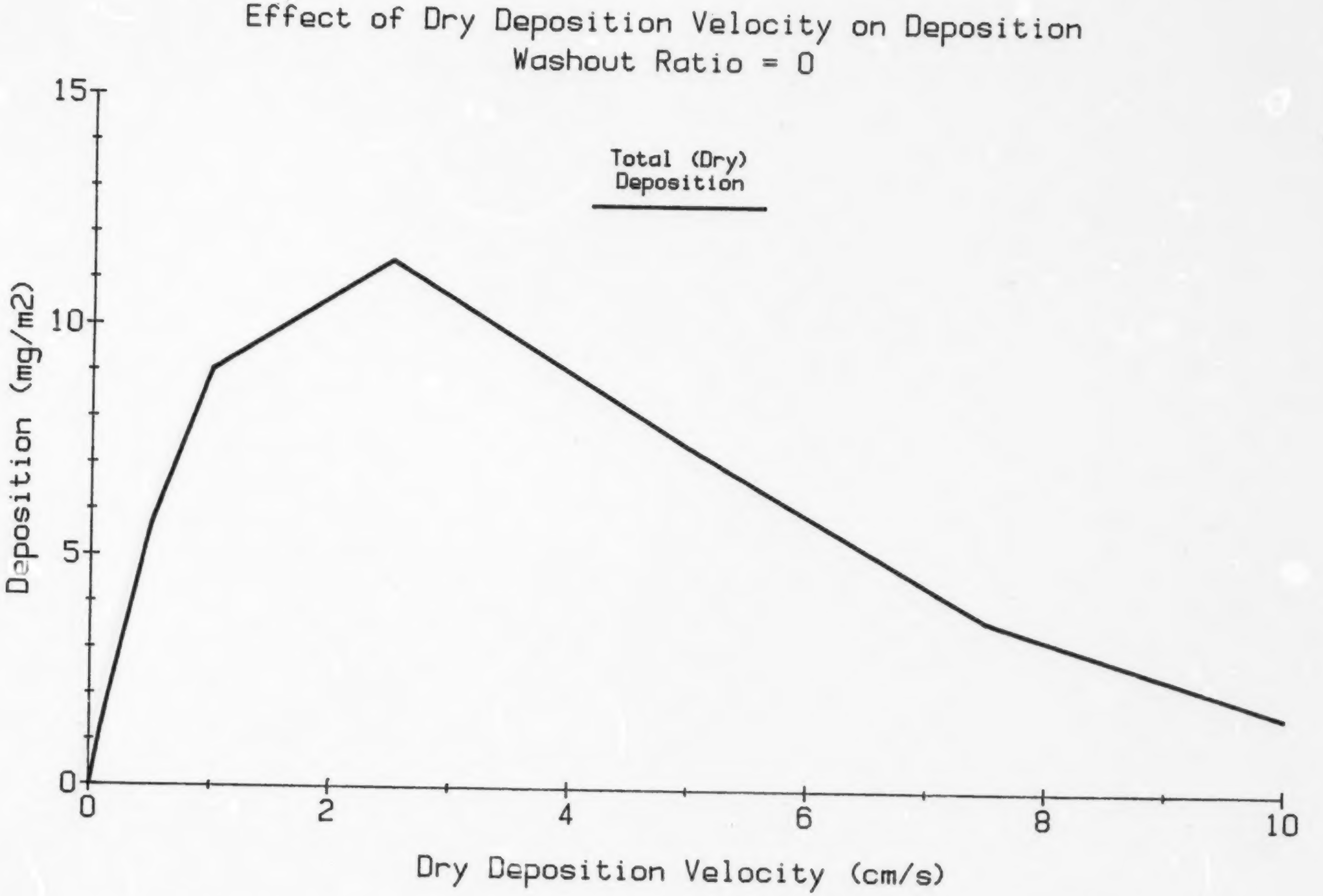

Figure 5.4 Sensitivity of atmostpheric deposition to dry deposition velocity (Washout ratio = 0).

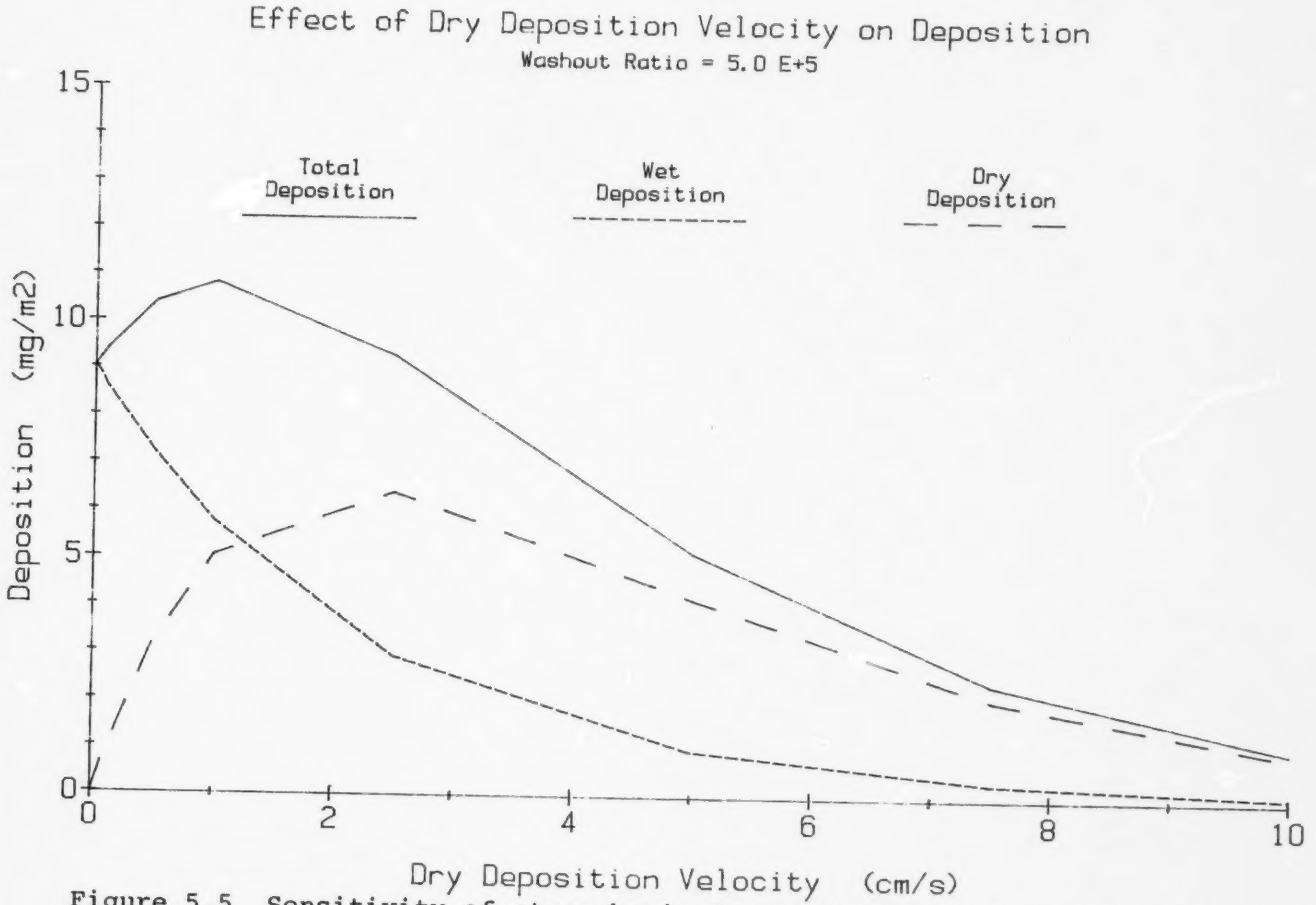

Figure 5.5 Sensitivity of atmospheric deposition to dry deposition velocity (Washout ratio = 5.E+5).

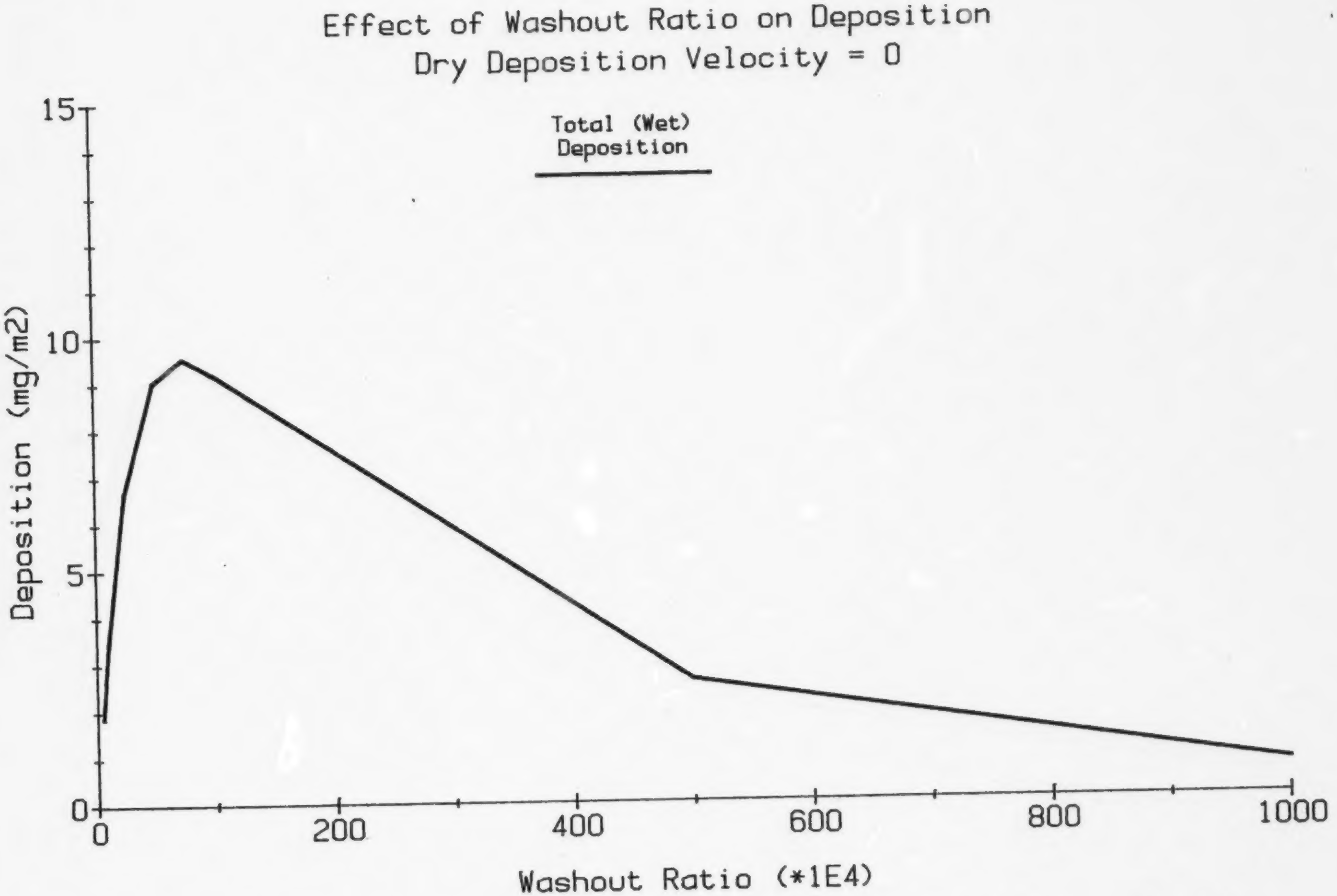

Figure 5.6 Sensitivity of atmospheric deposition to washout ratio (dry deposition velocity = 0).

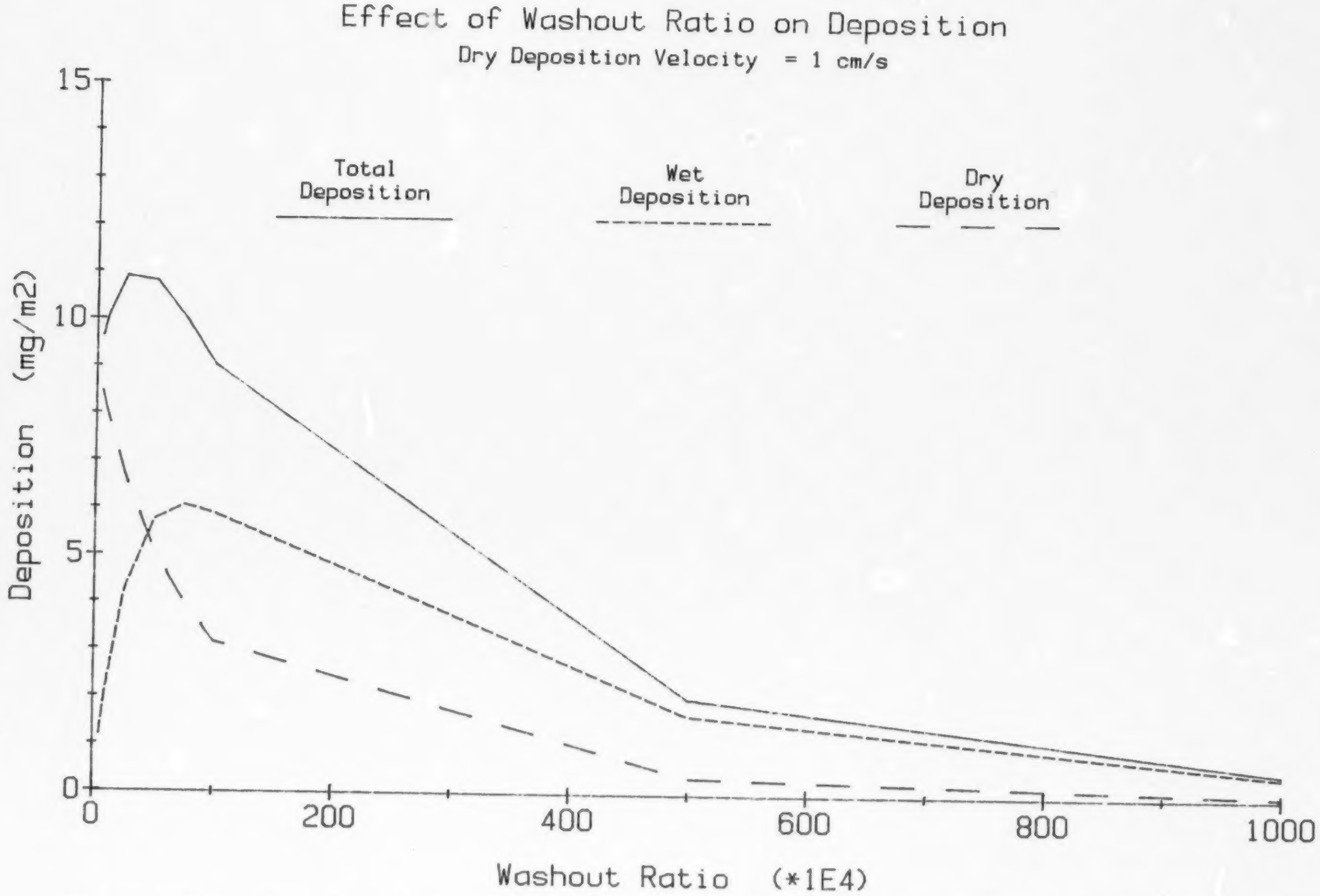

Figure 5.7 Sensitivity of atmospheric deposition to washout ratio (dry deposition velocity = 1 cm/s).

The generic environments in TOX-SCREEN are appropriate to screening. They serve to limit the input data required by the program, and also, to cause overpredictions (conservatism) of pollutant levels. Lack of simulation of a ground-water compartment results in the assumption of immediate transfer of "ground-water recharge" fluxes (computed by the soil model) into surface water. This scenario is unrealistic, and also de-emphasizs impacts on ground water.

SECTION 6

APPLICATION OF TOX-SCREEN TO SOUTHEAST OHIO STUDY AREA

The Southeast Ohio Study Area (SEOSA) was the object of data collection activities coordinated by the U.S. Environmental Monitoring Systems Laboratory (EMSL) in Las Vegas, Nevada. One purpose of the study was to collect data in several environmental media (air, water, soil, vegetation, etc.) to perform multimedia exposure assessment (Richitt et al., 1982). Examination of this data base showed that the spatial and temporal resolution was not adequate for detailed modeling application. However, we decided to apply TOX-SCREEN to the Southeast Ohio Study Area since the data base appears to represent the best multimedia data available. This application allowed us to exercise the full, multimedia capabilities of TOX-SCREEN on a "real-world" scenario and to compare results with observed data. We also used this application as the basis for the sensitivity tests of various model parameters; results of these sensitivity tests are described in the sections applicable to the model component tested. This section consists of a description of the SEOSA study area and data base, the TOX-SCREEN application, and comparison with observed concentrations.

6.1 DESCRIPTION OF SEOSA STUDY AREA AND DATA BASE

This description of the study area and associated data is based on conversations with EMSL personnel (R. Schonbrod, 1983), and three publications (Ritchett et al., 1982; Kolbow et al., 1983; Lockheed, 1984). The Southeast Ohio Study Area, shown in Figure 6.1, is a 525 km^2 basin situated along a 40 km stretch of the Ohio River, and includes areas in Kentucky, Ohio, and West Virginia. The area also contains a short stretch of the Big Sandy River. Urban area within the study area consists of the industrial cities Ashland, KY, Huntington, WV, and Ironton, OH; the total population is approximately 200,000.

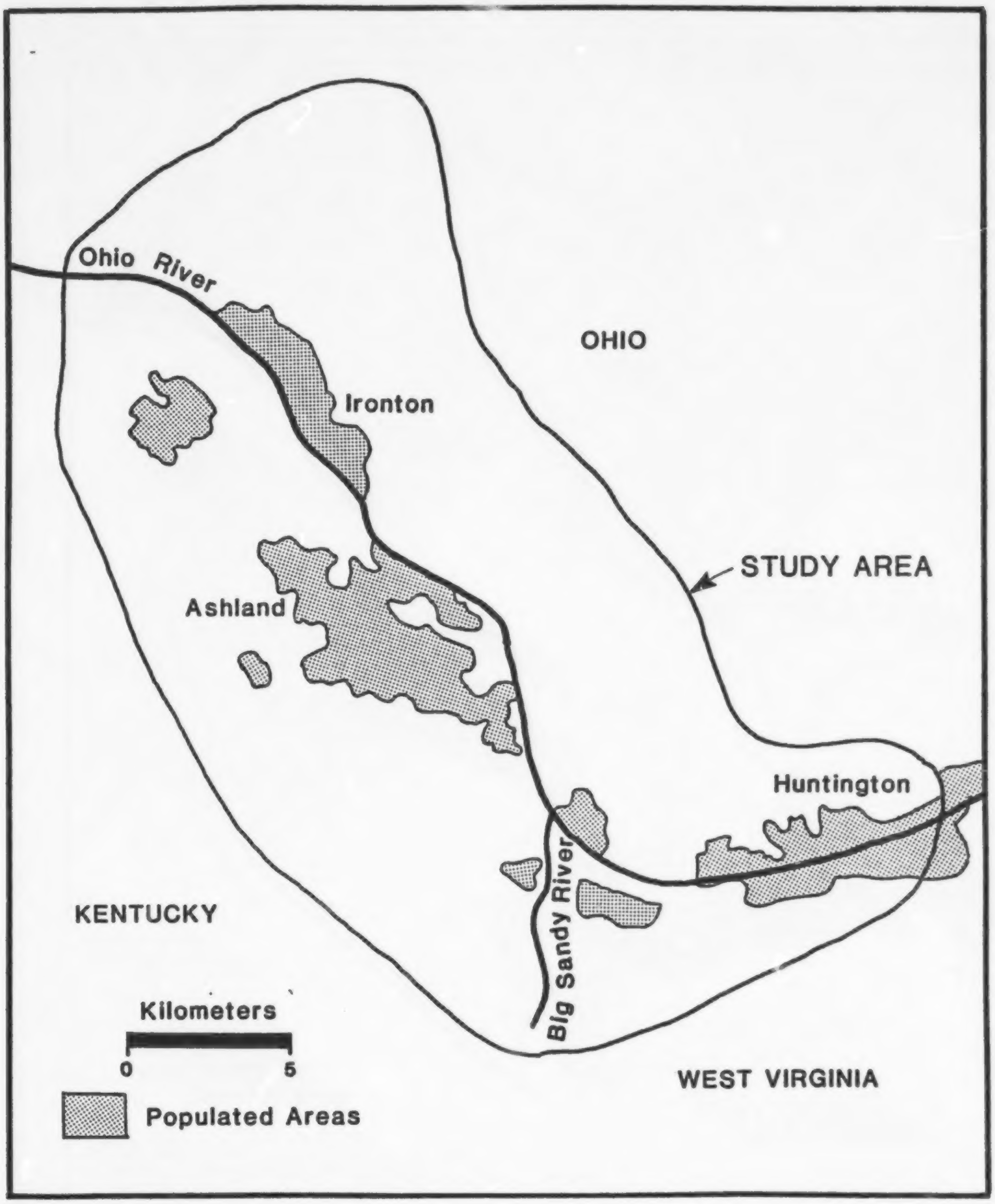

Figure 6.1 Southeast Ohio Study Area

Major sources of pollution in the study area are metallurgical and chemical industries which release pollutants to both air and water. There are coke plants, steel mills, a refinery, and chemical manufacturing plants. This heavy concentration of industrial activity in an isolated area was an important consideration in selection of the study area since most of the air pollution is due to internal sources. Data collection in the SEOSA included meterological data and concentrations of benzo(a)pyrene, benzene, chromium, cadmium, and arsenic in air, soil, surface water, sediments, and drinking water. In addition, an emissions inventory for benzo(a)pyrene was compiled.

The meterological data collection efforts were based on twelve stations which collected wind velocity and direction. Relative humidity and temperature were recorded at six of these stations, and a number of vertical temperature profiles were measured. The meteorological data were collected at approximately two-week intervals for two and one-half years.

Air pollution monitoring data for benzene, benzo(a)pyrene, cadmium, arsenic, and chromium were collected at two-week intervals at six of the meteorologic stations using various collection techniques and apparatus. All stations did not operate over the two-year period, and much of the data depends on total collected air volumes and estimated fractions of chemical recovered from filters during lab analysis. Consequently, the data are subject to significant uncertainty.

Concentrations of chemicals in soil and vegetation were determined in 4 grids over the basin consisting of about 75 separate points. Three small grids were spaced around the basin, and a larger grid covered a substantial portion of the area and was oriented along the river valley. Organics were sampled at about half of the points while metals were measured at all points. Depth profiles of chemicals were collected at one point in each grid. The depth profiles consist of 5 steps of 20 cm each for a total of approximately 110 cm. Data was collected twice, once in the fall of 1979 and again in the spring of 1980.

Concentrations in the river water and sediments were collected at approximately 12 points along the river in April, 1980, and again in March 1981, when the same points were sampled along with several additional sites emphasizing tributary inflows. The spring (March/April) is the time of high water in this river, and it was assumed that the maximum chemical load occurs at this time. Recently, EPA personnel associated with the sampling have had reason to doubt the validity of this assumption (Schonbrod, 1983). It was also concluded that the local sources of pollutant to the river - including point source pollutant discharges, nonpoint sources and deposition of air pollutants - had no significant impact on the measured pollutant levels (Schonbrod, 1983). Outflowing chemical concentrations were not significantly different from inflowing concentrations.

Emissions inventories for benzo(a)pyrene, cadmium, arsenic, and benzene were compiled for three years. These include significant industrial and institutional point sources, and area sources of pollutants.

6.2 MODEL APPLICATION

While this study area and associated data are not ideal for a critical comparison of model results with observed chemical concentrations, TOX-SCREEN was applied to the SEOSA area in order to exercise the complete multimedia capabilities of the model. The point sources of benzo(a)pyrene (for both air and water) are spread around the study area, while the generic environments assumed by TOX-SCREEN are designed for a single point source in each medium. TOX-SCREEN predictions exhibit no spatial resolution, so the observed data must be appropriately averaged for comparison. Also, the observed data are not well defined due largely to the low concentrations of BaP usually observed in the environment and the analytical problems discussed above. However, typical wind patterns in the valley approximate the constant wind direction assumed by the model. Wind directions tend to be oriented along the river valley. Also, the data monitoring frequency (bimonthly and annual) is generally compatible with TOX-SCREEN time resolution.

The TOX-SCREEN input was developed from the SEOSA data base (Lockheed, 1984) and related publications (Kolbow et al., 1983, Ritchett et al., 1982), National Weather Service data, Ohio River Valley Water Sanitation Commission (ORSANCO) data summaries, USGS data, and chemical references. A number of parameters were assigned the default values given by McDowell-Boyer and Hetrick (1982). The data collection effort is briefly described below, and Tables 6.1-6.4 list the final input set including parameter names, definitions, and values.

The scenario consists of a pollutant area source to air and a river with 10 reaches. Soil contaminated by the area source is adjacent to the river. While the study area actually contains many point and area sources of BaP, and thus is better suited to an area source scenario, a second scenario

TABLE 6.1 MODEL FLAGS AND AIR COMPARTMENT INPUT FOR SEOSA APPLICATION

Parameter	Definition	Value
AIRFLG	Signifies air point source	POIN (Run 1)
AIRFLG	Signifies area source to air	AREA (Run 2)
AIRPOL	Signifies pollutant is a particulate	PART
RIVER	Signifies a river is considered	YES
SEDRIV	Signifies sediment concentrations are input	YES
CHMFLG	Signifies pollutant is neutral	NONE
UW	Wind speed (m/s) (1/80 - 12/81)	3.1 2.9 4.0 4.0 2.8 2.8 2.4 2.4 2.3 2.9 3.3 3.2 3.5 3.5 3.7 3.9 2.9 2.8 2.7 2.6 2.9 2.9 2.9 3.3
UDG	Dry deposition velocity for gas	0.01 m/s
WRATG	Washout ratio for gas	6536.
AK	Pollutant degradation rate in air	0.0 /s
QS	Pollutant source rate to air	1.16E-4 kg/s
HMIX	Mixing height	927 m Run 1
HS	Stack height	50. m "
VG	Grav. settling velocity	0.0 m/s "
VS	Stack gas exit velocity	0.0 m/s "
SRAD	Stack radius	5.0 m "
RHO	Stack gas density	0.0 "
ENTPY	Stack gas enthalpy	0.0 "
CTYLTH	Length of area source	11648. n Run 2
UDP	Dry deposition velocity for particulate	7.5E-3 m/s
WRATP	Washout ratio for particulate	6.0E4

TABLE 6.2 RIVER COMPARTMENT INPUT FOR SEOSA APPLICATION

Parameter	Definition	Value
WKP	Photolysis rate constant	2.0E-6 /s
WKV	Volatilization rate constant	7.6E-8 /s
WKH, WKO, WKB	Hydrolysis, oxidation, and biological degradation rates	0.0
SWKSW	Soil-water partition coefficient	5.0E4 l/kg
WMINR	Pollutant loading rate	1.05E-5 kg/s
WVELR	River velocity (m/s) (1/80 - 12/81)	.55 .30 .34 .61 .61 .91 .52 .30 .37 .18 .24 .55 .24 .52 .67 1.2 .97 1.5 .52 .30 .37 .30 .43 .46
NR	Number of reaches	10
WLENR	Reach length	4000. m
WWIDR	Reach width	457. m
WDEPR	Reach depth	7.5 m
SEDCR	Sediment concentrations (mg/l) (1/80 - 12/81)	16. 16. 32. 62. 98. 200 200. 50. 25. 10. 14. 66. 12. 50. 38. 62. 98. 200 208. 50. 48. 39. 14. 10.

TABLE 6.3 SOIL COMPARTMENT INPUT (HYDROLOGIC PARAMETERS) FOR SEOSA APPLICATION

	Month											
Parameter	J	F	M	A	M	J	J	A	S	O	N	D
TA *	2.	1.	6.	12.	18.	22.	26.	26.	22.	12.	7.	3.
	1.	3.	6.	16.	16.	23.	24.	23.	19.	13.	7.	1.
NN	.94	.73	.80	.74	.71	.64	.58	.70	.75	.58	.64	.72
	.68	.72	.69	.77	.76	.71	.71	.61	.59	.64	.69	.82
S	.66	.61	.63	.60	.68	.69	.77	.81	.81	.71	.69	.67
	.65	.70	.61	.60	.76	.80	.80	.75	.72	.63	.64	.66
MPM	6.25	4.34	18.8	7.9	6.71	4.95	20.2	15.0	4.80	4.00	7.52	4.62
	1.63	10.7	4.19	13.6	13.2	15.0	9.25	2.62	4.06	6.43	3.12	6.63
MTR	.36	.27	.27	.19	.14	.08	.14	.10	.11	.25	.33	.39
	.22	.34	.22	.15	.14	.13	.13	.17	.27	.16	.14	.24
MN	13.	13.	22.	18.	16.	11.	14.	18.	10.	7.	10.	7.
	9.	15.	12.	21.	20.	19.	15.	5.	7.	12.	8.	18.
MT	30.4	(all months)										
L	38.0	(all months)										
A	0.26	(all months)										

---

* TA - Temperature (deg C)
NN - Cloud cover (frac)
S - Relative humidity (frac)
MPM - Total precipitation (cm)
MTR - Mean storm duration (days)
MN - Number of storm events
MT - Length of rainy season (days)
L - Latitude (deg)
A - Albedo (-)
for each parameter first line is 1980 data; second line is 1981 data

TABLE 6.4 SOIL COMPARTMENT INPUT (SOIL AND CHEMICAL PARAMETERS) FOR SEOSA APPLICATION

Parameter	Definition	Value
RS	Soil density	1.303 g/cm3
K1	Intrinsic permeability	5.E-11 cm2
C	Disconnectedness index	5.5
N	Effective porosity	0.35
OC	Organic carbon content	0.10 %
RDUST	Dust loading factor	100. ug/m3
SL	Solubility in water	3.8E-3 ug/ml
KOC	Organic carbon partition coefficient	6.4E5 l/kg
DA	Diffusion coefficient in air	0.05 cm2/s
KDE	Biodegradation rate	0.001 /day
H	Henry's Law constant	4.9E7 m3-atm/mol
MWT	Molecular weight	252. g/mol
VAL	Valence	0.
KNH,KBH,KAH	Hydrolysis rate constants	0.0
AR	Area of pollutant application	0.0 cm2
Z	Depth to ground water	11. m
DU	Depth of upper soil zone	30. cm
DM	Depth of middle soil zone	30. cm
FRN	Freundlich exponent	1.

was run in which a point source was considered rather than an area source. Since we wished to compare scenarios with equal areas of soil and water, and the soil area impacted by the point source plume is a computed quantity, it was necessary to first run the point source scenario. Then we ran the area source scenario with a total surface area equal to the soil and water areas impacted in the point source. The nature of these generic scenarios is described further in Section 5 and is shown in Figures 5.1 - 5.3.

The important meteorologic data necessary for this application are monthly values of wind velocity, temperature, humidity, cloud cover, and precipitation. These data were obtained from NOAA Daily Weather Data for Huntington, W.V. for 1980 and 1981. Also, soil data were taken primarily from SESOIL default data for a silt loam.

Data necessary to define the river system in this application are average depth and width, and monthly values of river velocities and suspended sediment concentrations. We decided to use observed sediment concentrations since the TOX-SCREEN algorithms for simulating that quantity do not operate at typical velocities for this section of the Ohio River. Since flow and suspended sediment data were not available from the SEOSA data base, they were obtained from ORSANCO data summaries and USGS publications, respectively.

The pollutant source term was adopted from Kolbow et al (1983). A constant BaP emission rate of 10 kg/day which consisted of 6 kg/day total from point sources and 4. kg/day total area source, was used. This estimated value could be refined significantly by more detailed analysis of the BaP emission inventory compiled as part of the SEOSA study.

A large fraction of all BaP in the SEOSA environment probably originates from internal sources, such as steel plants, coke ovens, chemical production, and other combustion activities; however, river water levels of this chemical result primarily from upstream sources (Richitt et al., 1982), with a small fraction resulting from local industrial discharge. To simulate representative water concentrations, we considered inputting a constant influent concentration (dissolved + adsorbed) of BaP to the study area of 0.055 ppb (Lockheed, 1984); however, we decided to assume an "initially clean environment " which is impacted only by local sources. The input source to water of 0.9 kg/day is based on an estimate by Kolbow et al. (1983).

The relatively high flow-through times for BaP in the air and surface water environments of the study area suggest that the simulated concentrations in these media respond rapidly, and reach steady-state conditions in a short time. However, for a chemical with a high adsorption coefficient, low degradation rate in soil, and continuous atmospheric deposition, concentrations in soil may increase steadily for years before reaching steady-state. As for the water, this suggests that one assume an existing BaP concentration in soil in order to accelerate attainment of steady-state conditions or simulate current levels. Also, the TOX-SCREEN soil model reports zero pollutant concentrations in soil until a threshhold value is reached. Preliminary runs of this scenario with an initially "clean" soil column, encountered this problem. We assumed an initial concentration in the moisture of the upper soil zone of 0.005 ug/ml in order to achieve the threshhold, but not approach observed levels in soil. This value actually resulted in an initial soil concentration of approximately 0.3 ug/kg, whereas measured values range from "0" to 5573 ug/kg and average 500 ug/kg. Thus the initial soil concentration is effectively 0.0 for comparison purposes.

Chemical parameters for BaP were (1) estimated from methods in Lyman et al. (1982); (2) obtained from previously published BaP modeling studies such as Kolbow et al. (1983), and Tucker et al. (1981); (3) obtained from Callahan et al. (1979); and (4) assigned default values from McDowell-Boyer and Hetrick (1982). While photolysis is a likely loss mechanism for BaP in air, the degradation rate was set to zero due to lack of an estimated value.

Predicted monthly BaP concentrations in air, water, and soil for the area and point source scenarios are shown in Table 6.5. Table 6.6 lists the predicted fluxes for the same time period. Some general trends are apparent in the results shown in these tables. First, the area source scenario predicts higher concentrations in all media, and corresponding higher intermedia fluxes. This tendency is not as large for water which is impacted primarily by the constant source term to the river. Given the fundamental differences between the two air dispersion models, this result is not unexpected. One possible cause for higher predictions in the area source scenario is the lack of plume depletion (by deposition) in this model compared to the point source model.

Second, while both air and water concentrations react rapidly to the monthly varying driving forces such as wind velocity, precipitation, and river flow, the soil concentrations increase constantly. This is caused largely by the low decay rate and high adsorption coefficient of BaP used in this application.

TABLE 6.5 BENZO(A)PYRENE CONCENTRATIONS PREDICTED FOR SOUTHEAST OHIO STUDY AREA

	Month											
	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
Air (ng/m^3)												
Area	45.	45.	43.	41.	55.	57.	59.	61.	55.	55.	55.	48.
Point	30.	27.	28.	25.	29.	29.	32.	35.	32.	32.	33.	29.
Water (dissolved + adsorbed) (ng/l)												
Area	15.	8.9	5.9	3.5	4.7	3.1	8.8	14.	11.	14.	9.4	8.7
Point	14.	7.1	5.4	3.2	4.0	2.5	7.4	12.	10.	12.	8.3	7.8
Soil (ng/g)												
Area	40.	42.	44.	46.	50.	53.	57.	60.	62.	65.	68.	70.
Point	20.	21.	22.	24.	25.	28.	29.	31.	32.	33.	35.	36.

TABLE 6.6 BENZO(A)PYRENE INTERMEDIA FLUXES PREDICTED FOR SOUTHEAST OHIO STUDY AREA

	MONTH											
	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
Deposition to Water (kg)												
Area	17.	21.	17.	20.	27.	29.	27.	23.	22.	23.	21.	21.
Point	11.	13.	11.	12.	15.	15.	14.	13.	13.	13.	13.	12.
Deposition to Soil (kg)												
Area	109.	138.	111.	132.	176.	189.	173.	151.	141.	150.	137.	132.
Point	71.	82.	71.	80.	94.	97.	93.	87.	83.	86.	82.	80.
Volatilization from Water (kg)												
Area	.208	.088	.064	.030	.020	.009	.016	.095	.101	.121	.183	.166
Point	.186	.079	.058	.027	.017	.008	.013	.081	.088	.105	.160	.146
Volatilization from Soil (kg)												
Area	.131	.057	.086	.047	.037	.033	.055	.138	.191	.187	.254	.203
Point	.065	.028	.044	.024	.018	.017	.028	.071	.098	.095	.130	.104
Surface Runoff (g)												
Area	.002	15.	.46	36.	51.	99.	27.	1.5	1.4	7.6	1.6	1.3
Point	.001	7.7	.23	18.	26.	51.	14.	.80	.70	3.9	.84	.68
Washload (kg)												
Area	.11	.12	.13	.13	.14	.15	.16	.17	.18	.19	.19	.20
Point	.056	.060	.064	.068	.072	.078	.083	.088	.092	.096	.099	.10

Averages of the measured concentrations of BaP in soil, water, and air (Lockheed, 1984) are shown in Table 6.7. The soil averages combine data for two sampling dates while the water data represent two sampling dates and various river/tributary locations in the basin. The air averages result from multiple sampling dates.

Figure 6.2 compares the simulated air concentrations with measured values for the Flatwoods station. This station recorded the highest BaP concentrations of the three "HI-VOL" recording stations due to its proximity to major sources and location with respect to dominant wind patterns in the basin (Richitt et al., 1982). The comparison shows that predicted concentrations were generally higher than measured by factors ranging from 65 to 0.8. for the point source, and 120 to 1.5 for the area source. As expected, the two simulated curves exhibit similar trends; however, their trend is opposite to that of the measured data.

Comparison of simulated and measured air concentrations is valid due to the fast flow-through time of the atmospheric system and lack of significant contribution from outside sources. However, as discussed above, the surface water BaP levels in the study area are due largely to sources external to the area, and are not represented in the simulation. Consequently, the underprediction of water concentrations by factors from 4 to 25 is understandable.

Simulated and measured average soil BaP concentrations vary by factors from 61 to 0.8 depending on simulation scenario (point or area source) and measurement site. The simulated soil BaP levels are steadily increasing, indicating that BaP may be accumulating in the soil faster than the rate of disappearance. Thus the simulation, which began with "zero" BaP concentration, is not directly comparable with observed data.

TABLE 6.7 MEASURED BENZO(A)PYRENE CONCENTRATIONS IN THE SOUTHEAST OHIO STUDY AREA (Lockheed, 1984)

Soil Concentration (ng/g)

	Site 1	Site 2	Site 3	Site 4
Average	240.	62.	1217.	491.
Maximum	1322.	125.	5267.	5573.
No. samples	11	10	11	49

Water Concentrations (ng/l)

	Ohio River	All Locations
Average	55.	59.
Maximum	171.	210.
No. samples	29	45

Air Concentrations (ng/l)

	Site FLA	Site HUN	Site SUN
Average	7.6	1.4	0.54
Maximum	34.	11.5	3.3
No. samples	23	44	42

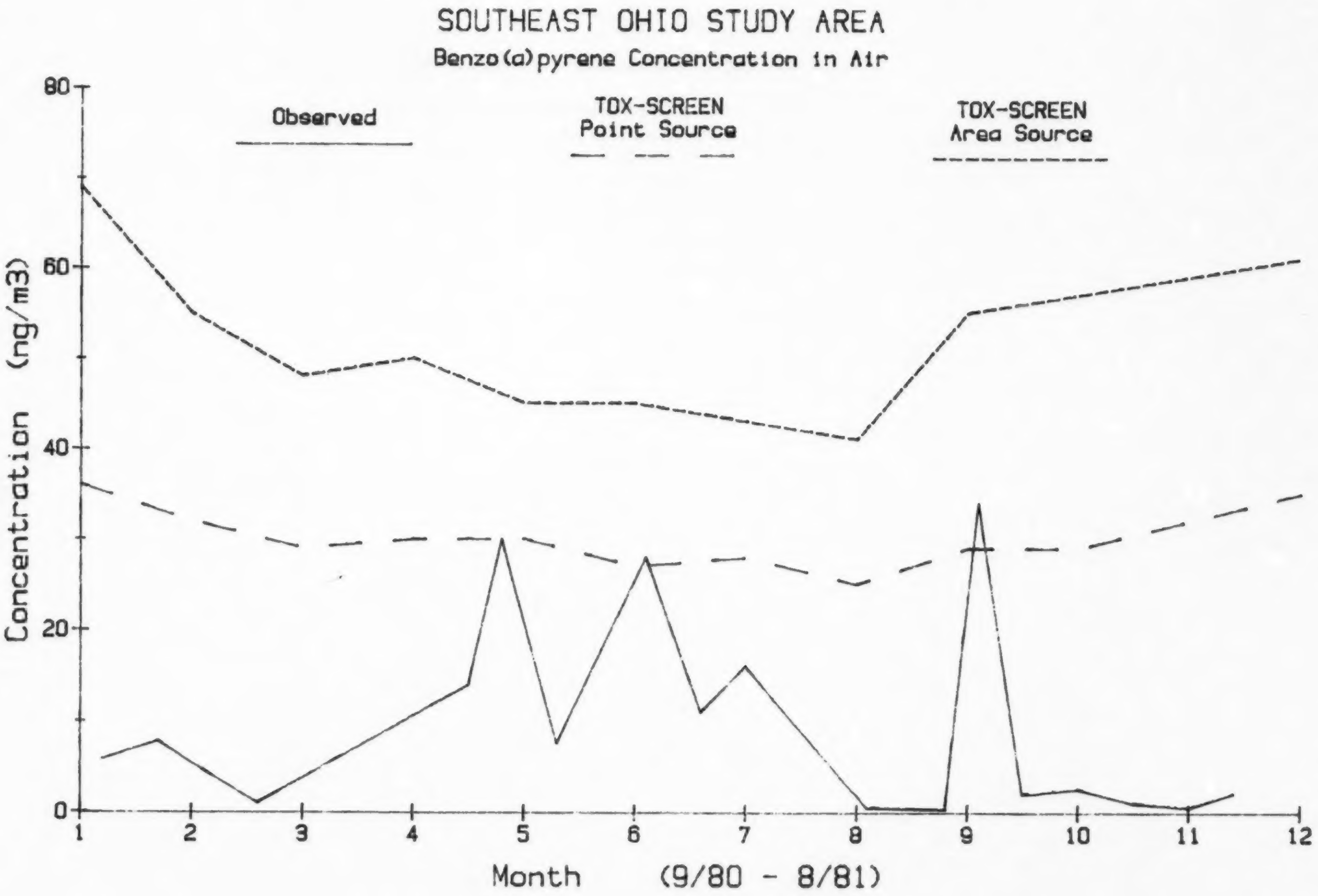

Figure 6.2 Comparison of observed and simulated air concentrations of Benzo(a)pyrene in the Southeast Ohio study area.

SECTION 7

TOX-SCREEN CODE AND DOCUMENTATION

Correct and efficient use of mathematical environmental models is facilitated by unambiguous operational procedures; thorough, accurate documentation; well documented and logical input formats; and output which is easy to interpret and contains all necessary simulation results. In addition, the code structure and programming techniques should facilitate understanding, debugging, and modification by persons other than the original developers.

The code, documentation, input, and output for TOX-SCREEN have been reviewed by Anderson-Nichols. For each of these subjects, a brief summary of what is available for TOX-SCREEN is presented along with a critique.

7.1 CODE

The TOX-SCREEN code consists of a main program and 26 subroutines. Fifteen routines were adapted from the SESOIL Model. The functions of the subroutines and the structure of the code are fairly well described in Chapter 3 of the User's Manual (Hetrick and McDowell-Boyer, 1984). Appendix A contains a listing of the FORTRAN variables and their definitions. Extensive use is made of common blocks to store FORTRAN variables and pass them around the program. The code also appears to be fairly well commented.

Based on the structure chart and subroutine descriptions, the code sections are based primarily upon the three separate media - air, water, and soil. The overall structure appears sound; however, the code logic is difficult to follow in some sections, particularly in the input routines and in computation of media interaction terms. We recognize the difficult task which the TOX-SCREEN developers faced with regard to (a) multimedia interaction terms between code sections for separate media, and (b) incorporating code from an outside source (SESOIL).

The following list contains several conclusions and recommendations regarding the code and its ease of interpretation, debugging, and understanding by other users.

1) Subroutines should be shorter and should perform closely related tasks only. For example, subroutine AIR is particularly long.

2) Branching within subroutines should be thoroughly commented, and principles of structured programming, such as indentation and standard structure figures, should be utilized.

3) Arguments to each subroutine should be described as "input", "output", or "modify".

4) Include statements could be used to incorporate common blocks into the code to reduce chances for error if the blocks are modified.

5) If possible, the media interaction terms should be better isolated in the code structure rather than computed within large subroutines for the individual media.

6) Under reasonable input scenarios, we sometimes experienced "system" execution errors due to underflows. These should be investigated and corrected where possible.

7.2 DOCUMENTATION

The TOX-SCREEN documentation consists of two separate documents. McDowell-Boyer and Hetrick (1982) documents the dispersion equations and interaction terms employed in the program, and Hetrick and McDowell-Boyer (1984) constitutes a "User's Manual" for the program. These two documents are abbreviated MBH and HMB in the discussion below.

MBH presents the theory for the air, aquatic, and intermedia component models in some detail, while referring the reader to the separately published documentation for SESOIL for the soil model (Bonazountas and Wagner, 1981). Appendices list model parameters and recommended default or typical values for selected parameters. HMB contains overviews of the model algorithms, description of the program structure, operational information, input data file description and formats, and descriptions of output produced by the program. Appendices contain a listing of program variables, sample input/output, and a code listing.

Generally, the TOX-SCREEN documentation package (MBH and HMB) provides the user with most of the information necessary to implement and operate the program. Use of the SESOIL User's Manual, while not necessary, is helpful. The TOX-SCREEN user's manual is logically organized and well written. Recommendations for correction of minor deficiencies in the documentation are itemized and discussed below.

1) MBH contains the typical and recommended default values for selected input parameters; this data should also be included in the User's Manual. Likewise, the methods for estimating bioaccumulation in food chains, which were added to TOX-SCREEN after publication of MBH, are documented in HMB.

2) In HMB, detailed instructions for using the program on DEC computers are presented in the body of the manual (e.g., Chapter 4.1, and Tables 1 and 2). These should be located in an appendix so as not to confuse users of other types of computers.

3) The IBM JCL found in Appendix B of HMB provides for the code to be recompiled with each execution of the model. This is generally not an efficient use of the machine resources. Separate IBM JCL streams should be provided to 1) compile and link the model, and 2) execute the model.

7.3 INPUT

TOX-SCREEN input parameter definitions and formats are described in Section 4.2 and Tables 1 and 3-9 of the User's Manual. The program reads the input from seven separate files during execution. These files contain the model flags, air, aquatic, soil, (3 files), and bioaccumulation input files.

The principal input documentation is contained in the user's manual. It is relatively easy to set up an input sequence from this information. More information such as maximum and minimum values and coded defaults where applicable should be included in the manual. As mentioned in Section 7.2, the typical values and user-default values contained in the appendices of MBH should be incorporated in the user's manual.

Tables 3-9 of the manual could also be ordered more logically (i.e., model flags, air, soil, water, bioaccumulation); and the correspondence between these tables and the respective input devices (files) should be clearly spelled out.

7.4 OUTPUT

TOX-SCREEN output is written to up to 7 separate output files depending on the water bodies considered in the simulation. The output contained in these files is documented in Chapter 5 and Appendix D of the user's manual.

Generally, the echoed input data and the SESOIL output tables are well organized and contain all important simulated results, i.e., compartment concentrations, storages, and pollutant fluxes for monthly and annual intervals. However, the TOX-SCREEN output tables titled "Monthly Pollutant Concentrations and Interaction Terms" should be modified to be similar to SESOIL monthly output, and the pollutant storages and net fluxes between media should be computed and output. It is recognized that this latter modification would be operationally difficult given the nature of the TOX-SCREEN air dispersion model and its media interaction algorithms; however, it would also allow pollutant mass balance checks to be computed. Also, as mentioned in Section 4, suspended sediment concentrations in rivers and lakes should be output.

SECTION 8

CONCLUSIONS AND RECOMMENDATIONS

8.1 SUITABILITY OF TOX-SCREEN FOR SCREENING

This evaluation of TOX-SCREEN has led to a number of conclusions regarding the capability of the model to perform reasonable screening assessments of chemicals with limited data availability. In this analysis, we considered an expected accuracy for screening methodologies of one order-of-magnitude. While testing included in this analysis primarily involved individual media, conclusions regarding the overall multimedia capabilities can be made from those tests as well as sensitivity testing and subjective review of the model. However, given the lack of multimedia data available to test this type of methodology, and the deliberate overpredictive nature of TOX-SCREEN, actual validation of the overall system is difficult.

Specific conclusions from this study were:

- The TOX-SCREEN model is currently an acceptable model for screening chemicals which do not adsorb to a large extent. Both the aquatic and soil models do not adequately consider adsorption in their transport simulations. High Kd pollutants in both media will tend to be advected out of the system too rapidly since bed sediments are not modeled in water bodies, and time of travel of soil pollutant to ground water does not depend on chemical properties.

- Testing of individual media models indicated that reasonable choice of input data resulted in predictions which satisfied the "one order-of-magnitude" criterion for screening accuracy in most cases. TOX-SCREEN may be on the boundary of acceptability based on this criterion.

- The air model requires careful attention because of its increased overpredictive potential (single wind direction). Testing results indicate less confidence that the one order-of-magnitude criterion will be satisfied.

- Predicted pollutant concentrations in rivers and lakes will generally be acceptable, based on testing results and analysis. Highly adsorbed chemicals will be questionable because of lack of a sediment bed and/or inappropriate simulation of suspended sediment concentrations.

- The soil model acceptability largely remains to be determined. Comparisons between SESOIL predictions and observed data were generally acceptable, but testing and analysis suggest deficiencies in soil layering, and the pollutant transport cycle.

- Individual process models, while necessarily simplified are generally based on current state-of-the-art mechanistic methods for fate/transport modeling. Empirical methods for some soil hydrologic processes and pollutant erosion processes are exceptions.

- All individual media models are relatively convenient to use, i.e., input data requirements are minimal, and typically available. The SESOIL model considers relatively more complex chemical processes, but these processes and associated input can generally be ignored, if desired.

- The code is somewhat confusing, and confirmation of "correct" operation is difficult. Mass conservation is a critical question in TOX-SCREEN; verification of mass balance should be incorporated. The documentation is appropriate.

8.2 RECOMMENDED CHANGES

A number of improvements in TOX-SCREEN have been identified in this study and are recommended for further consideration. We recognize that many of these recommended improvements would require significant effort to implement, and in some cases would slightly increase required user input. However, if TOX-SCREEN is to be applied to a wide spectrum of chemicals, more consideration of adsorption (aquatic and soil) should be included. The following list includes those recommended changes considered to be most important.

Atmospheric Dispersion Model

- Implement modification to buoyancy flux calculation as recommended by H.E. Cramer Co.
- Provide guidance to model users for avoiding errors caused by parameter sensitivity. This could include recommendations to test sensitivity of key parameters in all model applications.

Soil Model (SESOIL)

- Add additional layers to decrease the mathematical dispersion problems.
- Provide guidance to the user for avoiding errors caused by sensitivity to the soil disconnectivity parameter (C).
- Eliminate the threshhold which prevents "computation" of pollutant processes at low concentrations.
- Modify the pollutant cycle to include retardation in the computation of "time of travel" to ground water.
- Implement other necessary modifications recommended in the SESOIL testing program (Watson and Brown, 1984).

Aquatic Models

- Account for key water column-sediment bed interaction processes in lakes, rivers, and estuaries.
- Improve computation of suspended sediment concentration by accounting for low stream velocities.
- Correct the confusion regarding the lake velocity input parameter; refer to Section 4.1.2 for details.

Intermedia Transfer Models

- Provide additional user guidance for estimation of deposition parameters including table of values for representative and classes of chemicals.

Documentation/Code/Input/Output

- Improve user guidance for defaults since screening involves the use of uncertain data for new and poorly characterized chemicals. Also, correct inconsistencies in defaults between the User's Manual and the model algorithm documentation.

- Improve code structure (shorter subroutines, less complicated branching, indentation, etc.).
- Modify the output of information contained in "Monthly Pollutant Concentrations and Interactions Terms" to more closely resemble SESOIL output tables.

General

- Investigate the modifications and level-of-effort required to incorporate mass balance computations.
- Incorporate a simple ground-water model.
- Provide guidance for performance of sensitivity analysis as part of any assessment. Provide list of key sensitive parameters, and typical sensitivity ranges. This could also be incorporated into the code by allowing the user to enter a range of values for a parameter, and have the model compute the corresponding range of predictions.

REFERENCES

Bagnold, R.A. 1966. An Approach to the Sediment Transport Problem from General Physics, U.S. Geological Survey Professional Paper 422-I, U.S. Government Printing Office

Bass, A. 1980. Modeling Long-Range Transport and Diffusion. Preprint Volume for the Second Joint Conference on Application of Air Pollution Meteorology, American Meteorology Society, Boston, MA.

Bonazountas, M. and J. Wagner. 1981. "SESOIL: A Seasonal Soil Compartment Model," EPA/OTS Contract No. 68-01-6271, Arthur D. Little, Inc., Cambridge, MA.

Bonazountas, M., J. Wagner and B. Goodwin. 1982. "Evaluation of Seasonal/Soil Groundwater Pollutant Pathways via SESOIL," Final Draft Report, EPA/MDSD Contract No. 68-01-5949 (9), Arthur D. Little, Inc. Cambridge, MA.

Boutwell, S.H. 1982. Application of the Link-Node Models to the Transport and Fate of Copper in Newport Bay, CA. Paper for Environmental Quality Modeling (ECI244), Univ. of California, Davis, CA.

Bowers, J.F., J.R. Bjorklund and C. S. Cheney. 1979. Industrial Source Complex (ISC) Dispersion Model User's Guide, Volumes I and II. EPA Reports EPA-450/4-79-030 and 031 (NTIS Accession Numbers PB80-133044 and PB80-133051), U.S. Environmental Protection Agency, Research Triangle Park, NC.

Briggs, G.A. 1969. Plume Rise. Available as TID-25075 from Clearinghouse for Federal Scientific Technical Information, Springfield, VA.

Briggs, G.A. 1972. Chimney Plumes in Neutral and Stable Surroundings. Atmospheric Environments, 6(7) 507-510.

Briggs, G.A. 1973. Diffusion Estimates for Small Emissions, ATDL Contribution File No. (Draft) 79, Air Resources Atmospheric Turbulence and Diffusion Laboratory, Oak Ridge, TN.

Brooks, N.H. 1960. Diffusion of Sewage Effluent in an Ocean Current, in: Proceedings of the First International Conference on Waste Disposal in the Marine Environment, Pergamon Press.

Brooks R.H. and A.T. Corey. 1966. Properties of Porous Media Affecting Fluid Flow, Journ. Irrig. Div. Amer. Soc. Civil Eng. IR2, 61-88.

Burns, L.A., D.M. Cline and R.R. Lassiter. 1982. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation. U.S. Environmental Protection Agency, Athens, GA.

Callahan, M.A., M.W. Slimak, N.W. Gable, I.P. May, C.F. Fowler, J.R. Freed, P. Jennings, R.L. Durfee, F.C. Whitmore, B. Maestri, W.R. Mabey, B.R. Holt and C. Gould. 1979. Water Related Environmental Fate of 129 Priority Pollutants, Volumes I and II. Prepared for the U.S. EPA Office of Water Planning and Standards, Washington, D.C. by Versar, Inc., Springfield, VA. Available from NTIS. PB80-204373.

Carsel, R.F., C.N. Smith and M.N. Lorber. 1982. Pesticide Root Zone Model (PRZM) A Transient Hydraulic Model For Evaluating the Movement of Pesticides Within the Root and Lower Unsaturated Zones, User's Guide (Draft), Office of Pesticide Programs, HED/EFS, U.S. EPA, Washington, D.C.

Codell, R.B., K.T. Key and G. Whelan. 1982. A Collection of Mathematical Models for Dispersion in Surface Water and Ground Water. NUREG-0868. U.S. Nuclear Regulatory Commission, Washington, D.C.

Culkowski, W.M. and M.R. Patterson. 1976. A Comprehensive Atmospheric Transport and Diffusion Model. ORNL/NSF/EATC-17.

Ditoro, D.M., D. J. O'Connor, R. V. Thomann and J.P. St. John. 1981. Simplified Model of the Fate of Partitioning Chemicals in Lakes and Streams. Presented at the Workshop: "Modeling the Fate of Chemicals in Aquatic Environments." Pellston, MI.

Ditoro, D.M., J.J. Fitzpatrick and R.V. Thomann. 1982. Water Quality Analysis Simulation Program (WASP) and Model Verification Program (MVP) Documentation. U.S. Environmental Protection Agency, Duluth, MN.

Eagelson, P.S. 1978. Climate, Soil & Vegetation, Water Resources Research, Vol. 14, Nos. 1-7.

Eisenreich, S.J., B.B. Looney and J.D. Thornton. 1981. Airborne Organic Contaminants in the Great Lakes Ecosystem. Envir. Sci. Tech. Vol. 15. No. 1, 30-38.

Environmental Protection Agency. 1977. User's Manual for Single Source (CRSTER) Model. EPA-450/2-77-013, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Environmental Protection Agency, 1978. Guidelines on Air Quality Models. EPA 450/2-78-027 (AQPS No. 12-080), Office of Air Quality Planning and Standards.

Environmental Protection Agency. 1981. The Potential Atmospheric Impact of Chemicals Released to the Environment, Proceedings of Four Workshops (J.M. Miller, ed.) EPA 560/5-80-001.

Environmental Protection Agency. 1982. Testing for Field Applicability of Chemical Exposure Models, Results of the Workshop on Field Applicability Testing, Exposure Modeling Committee Report, March.

Farmer, W.J., M.S. Yang, J. Letey and W.F. Spencer. 1980. Land Disposal of Hexachlorobenzene Wastes: Controlling Vapor Movement in Soil, EPA-600/2-80-119, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH.

General Software Corporation (GSC). 1982. Graphical Exposure Modeling System (GEMS) User's Guide. Draft.

Gifford, F.A. and S.R. Hana., 1973. Modeling Urban Air Pollution. Atmospheric Environment, 7, 131-136.

Healy, J.W. 1980. Review of Resuspension Models, pp. 209-35 in Transuranic Elements in the Environment (W.C. Hanson, ed.), DOE/TIC-22800, U.S. Department of Energy, Technical Information Center.

H.E.C. 1983. Review of the Atmospheric Dispersion Model Component of the TOX-SCREEN Model, Technical Note prepared for Anderson-Nichols by H.E. Cramer Co., Inc. Salt Lake City, UT.

Hetrick, D.M. 1983a. ATM/TOX-SCREEN Comparisons. Draft Report.

Hetrick, D.M. 1983b. Comparison of Hydrologic Predictions by the SESOIL and AGTEHM Models. Draft Report.

Hetrick, D.M. 1983c. EXAMS/TOX-SCREEN Comparisons. Draft Report.

Hetrick, D.M. and L.M. McDowell-Boyer. Preliminary Validation Testing of TOX-SCREEN. (Informal Report).

Hetrick, D.M. and L.M. McDowell-Boyer. 1984. User's Manual for TOX-SCREEN: A Multimedia Screening-Level Program for Assessing the Potential Fate of Chemicals Released to the Environment. Oak Ridge National Laboratory, Oak Ridge, TN. (ORNL-6041) and U.S. EPA, Office of Toxic Substances, Washington, D.C. (EPA-560/5-83-024).

Hetrick, D.M., J.T. Holdeman and R.J. Luxmoore. 1982. AGTEHM: Documentation of Modifications to the Terrestrial Ecosystem Model (TEHM) for Agricultural Applications, ORNL/TM-7856.

Holzworth, G.C. 1972. Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States. Publication No. AP-101, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Johanson, R.C., J.C. Imhoff, H.H. Davis, Jr., J.L. Kittle, Jr. and A.S. Donigian, Jr. 1981. Users Manual for the Hydrological Simulation Program - FORTRAN (HSPF): Release 7. U.S. EPA Environmental Research Laboratory, Athens, GA.

Kincaid, C.T. J.R. Morrey, S.B. Yabusaki, A.R. Felmy and J.E. Rodgers. 1984. Geohydrochemical Models for Solute Migration, Volume 2, Preliminary Evaluation of Selected Computer Codes for Modeling Aqueous Solutions and Solute Migration in Soils and Geologic Media, EA-3417, Volume 2, Electric Power Research Institute, Palo Alto, CA.

Kolbow, D.H. Hikichi, C., Tuthill, C.W., Frank, G.B., Wiersma and R.D. Schonbrod. 1983. Kinetic Analyses:

Benzo(a)pyrene in Southeastern Ohio. Draft Paper submitted to Environmental Monitoring and Assessment.

Langbein, W.B. and S.A. Schumm. 1958. Yield of Sediment in Relation to Mean Annual Precipitation, Trans. Amer. Geophysical Union 39(6): 1076-84.

Laursen, E.M. 1958. The Total Sediment Load of Streams. Paper 1530, Proceedings of ASCE 84, HY1.

Leung, S.Y.T., R.V. Bulkley and J.J. Richard. 1982. Pesticide Accumulation in a New Impoundment in Iowa. Water Resources Bulletin, Vol. 18, No. 3, 485-493.

Lockheed Engineering and Management. 1984. Exposure Assessment Multimedia Monitoring System Database for Southeast Ohio. U.S. EPA Environmental Monitoring Systems Laboratory, Las Vegas, NV.

Lyman, W.J., W.F. Reehl and D.H. Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. McGraw Hill Co., New York, NY.

Mabey, W.R., J.H. Smith, R.T. Podoll, H. L. Johnson, T. Mill, T.W. Chou, J. Gates, I. Waight Partridge and D. Vandenberg. 1982. Aquatic Fate Process Data for Organic Priority Pollutants. Prepared by SRI International, Menlo Park, CA for U.S. EPA Office of Water Regulations and Standards, Washington, D.C.

McDowell-Boyer, L.M. and D.M. Hetrick. 1982. A Multimedia Screening-Level Model for Assessing the Potential Fate of Chemicals Released to the Environment. ORNL/TM-8334, Oak Ridge National Laboratory, Oak Ridge, TN.

McMahon, T.A. and P.J. Denison. 1979. Empirical Atmospheric Deposition Parameters - A Survey. Atmospheric Environment, Vol. 13., 571-585.

Mills, W.B., J.D. Dean, D.B. Porcella, S.A. Gherini, R.J.M. Hudson, W.E. Frick, G.L. Rupp and G.L. Bowie. 1982. Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants, Volumes 1 and 2. EPA 600/6-82-004 abc.

Mulkey, L.A., R.B. Ambrose Jr. and T.O. Barnwell, Jr. 1982. Aquatic Fate and Transport Modeling Techniques for Predicting Environmental Exposure to Organic Pesticides and Other Toxicants - A Comparative Study. U.S. EPA Environmental Research Laboratory, Athens, GA.

Orlob, G.T. 1981. Newport Bay, A Case Study of the Application of the Link-Node Hydrodynamic and Dynamic Water Quality Models. Prepared for Lowry and Associates, Irvine, CA.

ORNL. 1983. Multimedia Fate and Transport Modeling Project, Monthly Progress Report for October 1983, Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, TN.

ORSANCO. ORSANCO Quality Monitor. January 1981-December 1982. Ohio River Valley Water Sanitation Commission. Cincinnati, OH.

OTA. 1983. The Information Content of Premanufacture Notices Background Paper, Office of Technology Assessment, Washington, D.C.

Patterson, M.R., T.J. Sworski, A.L. Sjoreen, M.G., Browman, C.C. Coutant, D.M. Hetrick, B.D. Murphy and R.J. Raridon. A User's Manual for UTM-TOX, A Unified Transport Model. Draft. Prepared by Oak Ridge National Laboratory, Oak Ridge, TN, for U.S. EPA Office of Toxic Substances, Washington, D.C.

Penman, H.L. 1948. Natural Evaporation from Open Water, Bare Soil, and Grass, Proc. Royal Soc. of London, Ser. A. 193(1032),120-145.

Philip, J.R. 1969. Theory of Infiltration, in: Advances in Hydroscience, Vol.5, Ed. by V.T. Chow, pp 215-296, Academic Press, New York, NY.

Pritchard, D.W. 1969. Dispersion and Flushing of Pollutants in Estuaries. Journal of Hydraulics Division, ASCE. No HY1.

Rawn, A.M., F.R. Bowerman, and N.H. Brooks, 1960. Diffusers for Disposal of Sewage in Sea Water. J. Sanitary Eng. Div. Proceedings of the American Society of Civil Engineers, SA2: 65-89.

Ritchitt, P., V, Webb, R. Schonbrod. and J. Behar. 1982. Evaluation of a Multimedia Monitoring System in Southeast Ohio. Environmental Monitoring and Assessment (2)171-196.

Schnoor, J.L., A.R. Giaquinta, C. Sato, C.P. Robison, and D.B. McDonald. 1982. Refinement and Verification of Predictive Models of Suspended Sediment Dispersion and Desorption of Toxics From Dredged Sediments. Prepared for the GREAT River Environmental Action Team, U.S. Army Corps of Engineers, Iowa Institute of Hydraulic Research, Univ. of Iowa. IIHR Report NO 249.

Scott, B.C. 1981. Modeling of Atmospheric Wet Deposition. In: Atmospheric Pollutants in Natural Waters. S.J. Eisenreich, Ed., Ann Arbor Science, MI.

Shih, C.S. and E.T., Gloyna. 1970. Mathematical Model for the Transport of Radionuclides in Stream Systems. In: Environmental Surveillance in the Vicinity of Nuclear Facilities. Reinig, W.C., Ed. Charles C. Thomas Publishing Company, Springield, IL.

Shull, R.D., and E.T. Gloyna. 1968. Radioactivity Transport in Water-Simulation of Sustained Releases to Selected River Environments. EHE-04-6801, Technical Report No. 15 to the U.S. Atomic Energy Commission, University of Texas, Austin, TX.

Slinn, W.G.N., L. Hasse, B.B. Hicks, A.W. Hogan, D. Lal, P.S. Liss, K.D. Munnich, G.A. Sehmel, and O. Vittori. 1978. Some Aspects of the Transfer of Atmospheric Trace Constituents Past the Air-Sea Interface, Atmos. Environ. 12:2055-2087.

Southworth G.R. 1979. The Role of Volatilization in Removing Polycyclic Aromatic Hydrocarbons from Aquatic Environments, Bull. Environ. Contam. Toxicol. 21: 507-14.

Swann, R.L., P.J. McCall, and S. M. Unger. 1979. Volatility of Pesticides from Soil Surfaces, 177th National Meeting of the Am. Chem. Soc.

Task Committee on Preparation of Sedimentation Manual. 1971. Sediment Discharge Formulas. Journal of the Hydraulics Division, ASCE, Vol 97, No HY4. Proc. Paper No. 7786.

Tucker, W.A., A.Q. Eschenroeder and G.C. Magil. 1981. Air, Land, Water Analysis System (ALWAS). A Multimedia Model for Assessing the Effects of Airborne Toxic Substances on Surface Water Quality. Prepared by A.D. Little, Inc., Cambridge, MA. for U.S. EPA Environmental Research Laboratory, Athens, GA.

Turner, D.B. 1970. Workbook of Atmospheric Dispersion Estimates. Publication No. 999-AP-26, National Air Pollution Control Administration, Cincinnati, OH.

van den Honert, T.H. 1948. Water Transport in Plants as a Catenary Process, Trans. Faraday Soc. 3, pp 145-153.

van Genuchten, M.Th. and W.J. Alves. 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation, USDA, Technical Bulletin No. 1661, June.

Wagner, J., M. Bonazountas and M. Alsterberg. 1983. Potential Fate of Buried Halogenated Solvents via SESOIL, Arthur D. Little, Inc., Study in progress, Performed for the Office of Toxic Substances, EPA Contract No. 68-01-6271.

Watson, D.B. and S.M. Brown. 1984. Testing and Evaluation of the SESOIL Model. U.S. EPA, Environmental Research Laboratory, Athens, GA.

Yang, C.T. 1976. Minimum Unit Stream Power and Fluvial Hydraulics. Journal of the Hydraulics Division, ASCE, Vol. 102, No. HY7.

Yeh, G.T. and D.S. Ward. 1979. FEMWATER: A Finite Element Model of Water Flow Through Saturated-Unsaturated Porous Media, Oak Ridge National Laboratory. Report ORNL-5567.

Yeh, G.T. and D.S. Ward. 1981. FEMWASTE: A Finite Element Model of Waste Transport through Saturated-Unsaturated Porous Media, Oak Ridge National Laboratory. Report ORNL-5601.